乙二醇作为反应物的反应表19-14

说明：  
 Gibbs自由能判据: ‘1’代表从热力学角度利于反应正向进行；‘-1’代表从热力学角度不利于反应正向进行。  
 前线轨道理论判据: ‘1’代表基于前线轨道理论利于反应正向进行；‘-1’代表基于前线轨道理论不利于反应正向进行。  
 是否同时满足: ‘1’代表同时满足Gibbs和前线轨道理论判据，利于反应正向进行；‘-1’代表不同时满足上述两判据。  
 数据来源：所有原始属性数据计算方法均为 B3LYP/6-31G(2df,p)，单位均为eV。

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| --- | --- | --- | --- | --- | --- |
| 反应物A | 反应物B | 产物C | Gibbs自由能判据(ΔG) | 前线轨道理论判据 | 是否同时满足 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49458 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.74850) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44478 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.69871) | 1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10077 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-3.35470) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38569 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-2.63961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42770 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-2.68163) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55352 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-2.80745) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24444 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.49837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20708 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.46101) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04297 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.29689) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31737 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-1.57129) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78644 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.04037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29943 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.55336) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19396 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-1.44789) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83428 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.08821) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98473 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-1.23866) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26526 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.51918) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15546 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.40939) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99031 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.24424) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33328 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.58721) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.76001 HOMO: -6.64502 LUMO: 1.70343 factor:1 | -1 (0.98606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.89977 HOMO: -6.73754 LUMO: 1.60819 factor:1 | -1 (0.84630) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.46387 HOMO: -6.80829 LUMO: 2.45991 factor:1 | -1 (1.28220) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.03253 HOMO: -6.91713 LUMO: 2.43814 factor:1 | -1 (0.71354) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25496 HOMO: -6.60692 LUMO: 1.93745 factor:1 | -1 (0.49111) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.98244 HOMO: -6.26134 LUMO: 1.46125 factor:1 | -1 (0.76363) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11127 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.36520) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00863 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.26255) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08765 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.34158) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91853 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.17246) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17377 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.42770) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91659 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-2.17052) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78393 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-2.03786) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08995 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-2.34388) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60402 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.85795) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97861 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-1.23254) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54290 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.79683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04599 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.29992) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79674 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.05067) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94586 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.19979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51758 HOMO: -7.07768 LUMO: 2.48168 factor:1 | -1 (0.22849) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46709 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.72102) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40083 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.65476) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85695 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.11088) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42105 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.67498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94860 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-1.20253) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51027 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.76420) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56417 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-1.81810) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51160 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.76553) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60875 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-1.86267) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37746 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.63139) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91279 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.16672) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36946 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.62339) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51025 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.76418) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62095 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.87487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61213 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.86606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75529 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-1.00922) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37430 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.62823) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24573 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.49966) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27073 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.52466) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17207 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.42599) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21348 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.46741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05244 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-1.30636) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33424 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.58817) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04871 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.30264) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21151 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-1.46544) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33772 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-1.59165) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02405 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.27798) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54401 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.79794) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85199 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-2.10592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59851 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.85244) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82486 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-2.07879) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81574 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.06967) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37696 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-1.63089) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52020 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.77413) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22317 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.47710) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95470 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.20863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31035 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.56428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16148 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.41541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64703 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.90096) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73792 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-1.99185) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99675 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-2.25068) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98502 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-2.23895) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83904 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-2.09296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85917 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-2.11310) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63944 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.89337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73354 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.98747) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94432 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-2.19824) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94124 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-2.19517) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70980 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-2.96373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94225 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-2.19618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64493 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-2.89886) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41701 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-2.67093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35879 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-3.61272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66890 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-2.92283) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30257 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-3.55650) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27397 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-3.52790) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66082 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-2.91475) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58724 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-2.84117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20134 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-1.45526) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13127 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.38520) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32229 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-1.57622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16067 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-2.41460) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17730 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-2.43123) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28601 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-2.53994) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22688 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-2.48081) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13741 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-2.39134) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15120 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-2.40513) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30650 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-2.56043) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29023 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-2.54416) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48520 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-2.73913) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42632 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-1.68025) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19761 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.45154) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31843 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.57236) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41696 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-1.67089) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28772 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-2.54165) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27151 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-2.52543) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15553 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-2.40946) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98315 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-2.23708) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07534 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-2.32927) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92698 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-2.18091) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06247 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-2.31640) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13425 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-2.38818) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80573 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-2.05966) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76222 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-2.01615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92274 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-2.17667) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.33260 HOMO: -6.77019 LUMO: -1.17009 factor:1 | -1 (1.41347) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.73971 HOMO: -6.78652 LUMO: 1.35785 factor:1 | -1 (1.00636) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.64194 HOMO: -6.82734 LUMO: -0.68301 factor:1 | -1 (1.10413) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.86181 HOMO: -6.48175 LUMO: -2.19052 factor:1 | -1 (0.88426) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.80399 HOMO: -6.65863 LUMO: -0.77008 factor:1 | -1 (0.94209) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.99422 HOMO: -6.44094 LUMO: -2.20956 factor:1 | -1 (0.75185) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88810 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-2.14203) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83381 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-2.08774) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67144 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.92537) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42227 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.67620) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22222 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.47614) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47909 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.73302) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59890 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.85283) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90891 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-2.16284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44148 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-1.69541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21630 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.47023) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43380 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.68773) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96918 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-3.22311) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69246 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-3.94639) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00796 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-3.26188) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00858 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-3.26251) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03049 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-2.28442) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04018 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-2.29411) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56072 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.81465) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57865 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.83258) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81022 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-2.06415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69751 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.95144) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74548 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.99941) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74519 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.99912) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73844 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.99237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02093 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.27485) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66269 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.91662) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73060 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-1.98453) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68608 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.94001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81038 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-2.06431) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10647 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-2.36040) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06660 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-2.32053) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50253 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-2.75646) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29145 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-2.54538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69199 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-3.94592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94945 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-3.20338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88542 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-3.13935) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05103 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-3.30496) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37241 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-2.62633) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31907 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-2.57300) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64515 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-2.89907) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62427 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-2.87820) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72898 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-2.98291) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49418 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-2.74811) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82135 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-2.07528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59128 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.84520) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70456 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-1.95849) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27442 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-2.52835) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30038 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-2.55431) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34892 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-2.60285) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41896 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-2.67289) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46185 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-2.71578) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08145 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-3.33538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55899 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-2.81292) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57339 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-2.82732) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82935 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-2.08328) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30618 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.56011) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06991 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.32383) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23943 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-1.49336) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45699 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-1.71092) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12783 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-2.38176) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87408 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-2.12801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14274 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-2.39667) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28950 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-1.54343) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20879 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.46272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38118 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.63510) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27489 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.52882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06426 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-2.31819) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93106 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-3.18498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58974 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-2.84367) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33284 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-2.58677) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58006 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-2.83398) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54080 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.79473) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30346 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.55739) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22969 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.48362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25663 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.51056) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53703 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.79095) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60666 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.86059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49866 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.75259) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90478 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-2.15871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13104 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-2.38497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03860 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-2.29253) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09429 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.34822) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97992 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-1.23385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12291 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-1.37684) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17334 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.42726) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14746 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.40139) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95717 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.21110) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09821 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-1.35213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18977 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.44370) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07233 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-1.32626) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85270 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.10663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09002 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-1.34394) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23383 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-1.48776) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72370 HOMO: -6.06542 LUMO: 1.92112 factor:1 | -1 (0.02237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06676 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.32069) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06589 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.31982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37568 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-1.62961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38534 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.63927) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33481 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.58874) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42983 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-1.68376) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73961 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.99353) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48268 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.73660) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61705 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.87097) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39813 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.65206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50325 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.75718) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06675 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-1.32068) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38412 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.63805) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41468 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.66861) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36007 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-0.61400) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47436 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-0.72829) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37904 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.63296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48712 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-0.74105) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98576 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-2.23969) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93648 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-2.19041) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66360 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-2.91752) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16399 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-3.41791) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37064 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-2.62457) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64139 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-2.89532) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52275 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-2.77668) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28561 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-1.53954) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47897 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.73290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38833 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-1.64226) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54627 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-1.80020) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54053 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.79445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61214 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-2.86607) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55946 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-2.81339) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69067 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-2.94460) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85612 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-3.11004) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98592 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-2.23985) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15017 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-2.40410) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18065 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-2.43458) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09112 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-2.34505) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15532 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.40925) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23058 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-2.48451) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43769 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-2.69161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48079 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-2.73472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49722 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-2.75115) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57568 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-1.82961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65408 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-1.90801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67111 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-1.92504) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79294 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-2.04687) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04331 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-2.29724) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86744 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-2.12137) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85085 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-2.10477) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24663 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-2.50056) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15235 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-2.40628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69125 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-1.94518) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99964 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-2.25357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24971 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-2.50364) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14486 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-2.39879) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23491 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-2.48883) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35331 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-1.60724) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45740 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-1.71132) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51408 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-1.76801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26456 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-3.51849) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.79654 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-4.05047) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88970 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-2.14363) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73239 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-2.98631) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95523 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-2.20916) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01655 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-3.27048) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02148 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-3.27541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67348 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.92741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79010 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-3.04403) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87712 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-3.13105) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67666 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-2.93058) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09404 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-1.34797) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29402 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-1.54795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46123 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-1.71516) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07711 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-2.33104) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10133 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-2.35525) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05740 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-3.31133) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06771 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-3.32164) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83263 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-3.08656) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03432 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-3.28825) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81449 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-2.06842) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56882 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-2.82275) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63334 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-2.88726) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55987 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-2.81379) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63687 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-2.89080) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71373 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.96766) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51805 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-1.77198) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90940 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-3.16332) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49900 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.75293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11683 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-3.37076) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50830 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-2.76223) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00301 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-2.25694) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78853 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-2.04246) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84905 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-2.10298) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00337 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-2.25729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89202 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-2.14594) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60017 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.85410) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49653 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.75045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82197 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-2.07590) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70782 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.96175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21869 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-2.47262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10613 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-3.36006) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71951 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-2.97344) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78671 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-2.04064) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64517 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-2.89910) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60973 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-1.86365) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90929 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-3.16321) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64686 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-2.90079) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39879 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-3.65272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21767 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-3.47160) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65964 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-3.91357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05405 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-3.30798) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39336 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-2.64729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19150 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-3.44542) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46035 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-2.71428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67647 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-2.93039) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27958 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-3.53351) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56904 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-2.82296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87462 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-3.12855) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50503 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-2.75896) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54738 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-2.80130) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22505 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-3.47898) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.63341 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-3.88734) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01955 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-3.27348) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72996 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-2.98389) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24886 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-3.50279) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82044 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-3.07437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76223 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-4.01616) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21109 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-3.46502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44846 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-2.70239) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67249 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-2.92642) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01049 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-3.26441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93076 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-3.18468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58572 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.83965) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69427 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-1.94820) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07992 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-1.33385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11995 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-1.37388) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19489 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-1.44882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32441 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.57834) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21121 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-1.46514) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24539 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.49932) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46676 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-1.72068) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42501 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.67894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29233 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.54626) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09435 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-3.34828) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90934 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-3.16327) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26282 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-3.51675) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10091 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-3.35484) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25979 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-1.51371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36126 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-1.61519) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96746 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-3.22139) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89008 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-3.14400) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85878 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-3.11271) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01157 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-3.26550) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42151 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-3.67544) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38778 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-2.64171) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51769 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-2.77162) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56836 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-2.82228) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39576 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-1.64969) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37908 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-1.63301) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18229 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.43622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04596 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.29989) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06852 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.32245) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40477 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-1.65870) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15198 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.40590) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58417 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-2.83809) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69472 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-2.94865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60821 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.86214) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71755 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.97147) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86827 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-1.12220) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35997 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-2.61390) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50648 HOMO: -6.65863 LUMO: -0.57416 factor:1 | -1 (0.23960) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45170 HOMO: -6.49808 LUMO: -0.54695 factor:1 | -1 (0.29437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52985 HOMO: -6.50080 LUMO: -0.61498 factor:1 | -1 (0.21622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94292 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.19685) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99334 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.24727) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04610 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.30003) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17250 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.42643) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28241 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.53634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83026 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-3.08419) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90181 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-2.15574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82807 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-2.08200) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92007 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-2.17400) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58747 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.84139) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48776 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.74169) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48123 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.73516) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63514 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.88907) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43068 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.68461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36263 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.61656) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34407 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.59800) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36992 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.62385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48851 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.74244) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49945 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.75337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72660 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.98053) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59611 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-2.85004) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85041 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-2.10434) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82045 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-2.07438) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84815 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-2.10208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95907 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-2.21299) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70271 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-1.95663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81718 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-2.07111) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77264 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-2.02657) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42150 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-2.67542) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20660 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.46053) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32595 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.57987) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49093 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.74486) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45540 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-2.70933) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07439 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-2.32832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37684 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-2.63077) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40079 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-2.65472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46977 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-2.72370) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48882 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-2.74274) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48155 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-2.73548) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68670 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-2.94063) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64826 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.90218) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83879 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-2.09272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58170 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-1.83563) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65916 HOMO: -6.32665 LUMO: 1.87759 factor:1 | -1 (0.08691) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99925 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.25317) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72542 HOMO: -6.72665 LUMO: 2.12521 factor:1 | -1 (0.02065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25294 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.50687) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52590 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.77982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53566 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.78959) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79151 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.04543) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58475 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.83868) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60285 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.85678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99878 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-1.25270) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58160 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.83553) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05501 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-2.30894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20696 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-2.46089) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98619 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-2.24012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09477 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-2.34870) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91052 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-2.16445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17137 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-2.42530) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12889 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-2.38282) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34222 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-3.59615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37134 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-2.62527) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54574 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-2.79967) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59867 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-2.85260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31872 HOMO: -7.09129 LUMO: 2.10344 factor:1 | -1 (0.42735) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33774 HOMO: -6.77564 LUMO: 2.14970 factor:1 | -1 (0.40833) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49222 HOMO: -6.81645 LUMO: 1.85854 factor:1 | -1 (0.25386) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81957 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.07350) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76198 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-1.01591) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85815 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-1.11207) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09856 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.35249) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91216 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.16609) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21528 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.46921) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20788 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.46180) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34761 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.60153) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62114 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.87506) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94226 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.19619) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86185 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.11578) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06604 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.31997) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86830 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.12222) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32193 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-2.57586) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.49270 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-3.74663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49399 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-2.74791) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58011 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-2.83404) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50931 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-2.76323) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45951 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-2.71344) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15578 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-2.40970) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34451 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-2.59844) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38832 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.64225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20337 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.45730) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04032 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-2.29425) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24258 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-2.49651) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40218 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-2.65610) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10495 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-2.35887) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98478 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-2.23871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17409 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-2.42802) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97969 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-2.23362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57048 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-2.82441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25904 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-2.51297) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49728 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-2.75121) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40598 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-2.65991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25990 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.51382) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45922 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.71315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09978 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.35371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85085 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.10478) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09785 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.35178) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97586 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-1.22979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32876 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-2.58269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23677 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.49069) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49718 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-1.75111) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53933 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.79326) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12870 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-2.38263) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98889 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-2.24282) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14535 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-2.39928) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08973 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-2.34366) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39291 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-3.64684) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00257 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-3.25650) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87622 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-3.13015) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02689 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-3.28082) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18616 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-3.44009) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98319 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-3.23712) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51291 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.76684) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70505 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.95897) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55480 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-2.80873) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77013 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-3.02406) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22487 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.47880) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56240 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.81633) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73530 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-2.98923) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36323 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-3.61716) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81527 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-3.06920) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56047 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-1.81440) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82116 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-2.07509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49529 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-2.74922) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67619 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-2.93012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42246 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.67638) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47661 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.73054) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66074 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-2.91467) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84741 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-3.10134) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41735 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-3.67128) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23718 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-3.49111) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59592 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-2.84985) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72009 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-2.97401) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74888 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-3.00280) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24384 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-1.49777) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21456 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.46849) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01869 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.27262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33171 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.58563) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17731 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.43124) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15091 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.40484) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72618 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-2.98011) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85497 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-3.10890) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92858 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-3.18251) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07842 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.33235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18961 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.44354) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15502 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.40895) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25470 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.50863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23489 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.48882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39960 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.65353) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19657 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.45050) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15475 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-1.40868) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09113 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.34506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67064 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-2.92457) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79671 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-3.05064) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04700 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-3.30093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59826 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-2.85219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71375 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-2.96767) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94980 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-3.20373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62978 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.88371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11366 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.36759) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00963 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.26356) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21881 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.47273) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21696 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-1.47088) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24512 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.49905) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12199 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.37592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79370 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.04763) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12674 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-2.38067) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49868 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.75260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73313 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.98706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84363 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-2.09756) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05099 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-2.30491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49545 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-0.74937) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70821 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.96214) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51128 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.76521) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44428 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.69821) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26410 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-2.51803) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63876 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.89269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63601 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.88994) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28689 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.54082) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51187 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-1.76580) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60522 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.85915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71978 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.97371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72789 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.98181) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83094 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.08486) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66489 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.91882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45028 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.70420) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74726 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.00119) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73322 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.98715) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74024 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.99417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64182 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.89574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35748 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.61141) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64342 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.89735) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74353 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-0.99746) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86375 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.11768) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71523 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-0.96916) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75610 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-1.01003) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85347 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-1.10739) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80340 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-1.05733) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72998 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.98391) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65490 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-0.90883) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36347 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.61740) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65074 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.90467) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57316 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.82709) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59665 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.85057) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65333 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.90725) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79295 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.04688) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32741 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.58134) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38278 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.63671) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22006 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-1.47399) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14806 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.40199) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72965 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.98357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52280 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-2.77673) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77011 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-2.02404) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59253 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.84646) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86644 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-2.12037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67959 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.93351) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68568 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.93961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65186 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.90579) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49262 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.74654) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57564 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.82957) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41468 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.66861) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89713 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-2.15106) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62038 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-2.87431) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54083 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.79476) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22766 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.48159) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26898 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-2.52290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30006 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.55399) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53944 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-1.79337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02815 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-2.28208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96200 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-2.21593) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44424 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-2.69817) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88956 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-3.14349) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53402 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-1.78795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73054 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-1.98447) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15417 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-2.40810) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06402 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-2.31795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11044 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-2.36437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58150 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-2.83543) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71920 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.97312) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85144 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-2.10537) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30838 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-2.56231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83013 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-3.08406) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77398 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-1.02791) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62934 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-1.88327) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78691 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.04084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56488 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.81881) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48727 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-1.74120) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75144 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-2.00537) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32794 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-2.58187) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79242 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-2.04635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78463 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-3.03856) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.56791 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-3.82184) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71867 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-2.97260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57376 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.82769) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45255 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-1.70648) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91031 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.16424) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31274 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.56667) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14459 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-2.39852) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59998 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.85391) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05838 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-3.31231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78569 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-3.03962) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37241 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.62634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27377 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.52770) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14190 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-2.39583) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58211 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-1.83603) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39564 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-3.64956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82901 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-3.08294) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11879 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-3.37272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61222 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-2.86615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39517 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-3.64910) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81040 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-3.06433) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73634 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.99027) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68929 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.94322) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41045 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-2.66438) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30498 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-2.55890) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88290 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-2.13683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67992 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-2.93385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67609 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-2.93001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24479 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.49872) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43684 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-2.69077) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30813 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-2.56206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48404 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.73796) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67471 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.92863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27524 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-1.52917) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68600 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.93993) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20821 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-2.46214) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28811 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.54204) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51141 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-1.76534) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04942 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-1.30334) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50745 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.76137) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19479 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.44872) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21520 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.46912) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50473 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.75865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38973 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.64366) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10034 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.35427) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06635 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.32028) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36704 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.62096) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09277 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.34670) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87007 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.12400) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40851 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.66243) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27525 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.52918) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09855 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-2.35248) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68461 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.93854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73820 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.99213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35923 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.61315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60891 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-1.86284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70028 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-1.95421) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31312 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-1.56705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32116 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.57509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33705 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.59098) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04213 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.29606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51107 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.76499) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57364 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-1.82757) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64875 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-1.90267) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24395 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-1.49788) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48942 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-1.74335) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65460 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-1.90852) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29119 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-1.54512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61484 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.86877) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74644 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-2.00036) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37184 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-1.62577) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40063 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-1.65456) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51628 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-1.77021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09442 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-1.34835) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30899 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.56291) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80627 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-2.06020) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39163 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-1.64555) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06759 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-1.32152) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93365 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-2.18758) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94383 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-2.19775) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68861 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.94254) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55218 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.80611) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59115 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.84508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23128 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.48521) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76000 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.01392) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61838 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-1.87231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66151 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-1.91544) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32044 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-1.57437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93262 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-2.18654) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16247 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-2.41640) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72399 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-1.97791) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49772 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-1.75165) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75079 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-2.00472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37037 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-1.62430) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25309 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.50702) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35410 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.60803) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11989 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.37382) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37672 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.63065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56326 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.81719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16105 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.41497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59803 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.85196) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38619 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.64012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43098 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.68491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09468 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.34861) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53096 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.78489) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55166 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-1.80558) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66603 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-1.91995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41100 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.66493) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49024 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-1.74417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27534 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-2.52927) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58004 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.83397) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31347 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.56740) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21685 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.47078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29443 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.54836) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07608 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.33001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67653 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-1.93046) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36235 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.61627) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10504 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.35897) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31566 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.56959) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73631 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-1.99024) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43691 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-1.69083) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71852 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.97244) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40345 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-2.65738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45786 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.71179) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19097 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-1.44490) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94533 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.19926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56668 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.82060) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31924 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.57317) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45582 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.70975) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26953 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.52346) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10575 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.35968) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26216 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.51609) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04619 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.30011) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70165 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.95557) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30468 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-2.55860) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43549 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.68942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03504 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-2.28897) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12177 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-1.37570) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31590 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.56982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08299 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.33692) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11815 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.37208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29045 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.54438) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92086 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-2.17479) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15325 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-1.40718) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09668 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.35061) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31165 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.56558) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48181 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.73574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50298 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.75691) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25775 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.51168) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56122 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.81514) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72840 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.98233) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68701 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.94094) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31539 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.56932) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89827 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.15219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00670 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.26063) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.77304 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-0.02697) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25920 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-0.51313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.13765 HOMO: -6.63686 LUMO: 2.09800 factor:1 | -1 (0.60842) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35733 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (0.38874) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.07180 HOMO: -6.37019 LUMO: 2.35923 factor:1 | -1 (0.67427) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67802 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (0.06806) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.36089 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (0.38518) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49902 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (0.24705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.20353 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (0.54254) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25123 HOMO: -6.72121 LUMO: 1.33608 factor:1 | -1 (0.49484) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64287 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.89680) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20375 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-2.45768) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77174 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-2.02567) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59740 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-1.85133) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86190 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.11583) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56312 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.81705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10430 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-1.35823) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81866 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.07259) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36129 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.61522) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64035 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-0.89427) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20573 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-0.45965) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86860 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-1.12252) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76586 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-2.01979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48327 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-1.73720) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78840 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-2.04232) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53299 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-1.78692) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62246 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.87639) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44752 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.70145) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63601 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-1.88994) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15154 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-1.40547) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63971 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.89364) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80863 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-3.06256) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86656 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-3.12049) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49039 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-2.74432) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00483 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-3.25875) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.77681 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-4.03074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11209 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-3.36602) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76346 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-3.01739) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67866 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.93259) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72838 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-0.98230) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76359 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-1.01752) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50788 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.76181) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71208 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.96600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57618 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.83011) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21582 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-0.46975) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98827 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.24220) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99091 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-1.24484) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61050 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.86442) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49961 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.75354) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12537 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-3.37930) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13909 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-3.39301) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76352 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-3.01744) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37615 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.63008) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65390 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-0.90783) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52432 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.77825) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15707 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.41100) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74095 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.99488) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25512 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.50904) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38168 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.63560) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46173 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.71566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12474 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.37866) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13350 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.38743) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.62656) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63858 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.89251) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13699 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.39092) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48195 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.73588) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11065 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.36458) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46647 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.72039) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31386 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.56779) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72628 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.98021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68207 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-2.93600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65466 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.90859) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36431 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.61824) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59714 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.85106) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50402 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.75795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24701 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.50093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50677 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.76069) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67471 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.92864) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63501 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.88894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31637 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.57030) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39086 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-2.64478) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44742 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-0.70135) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40965 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-0.66358) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09598 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.34991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41569 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.66962) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87845 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.13237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96345 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-1.21738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58802 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.84195) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48724 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-2.74117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19783 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-1.45175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15244 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.40637) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10248 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.35641) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31084 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.56476) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25107 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-2.50500) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57290 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-2.82683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13985 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.39378) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50883 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-0.76276) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81148 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.06541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70323 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-0.95716) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47117 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-0.72510) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71685 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-2.97078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44274 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-0.69667) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49430 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-0.74823) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57474 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-0.82867) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44725 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-0.70118) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27686 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.53079) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59507 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.84900) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38756 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-2.64149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23695 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-2.49088) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56536 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-2.81929) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12885 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.38277) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22966 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.48359) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13404 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.38797) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79341 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.04734) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13949 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.39341) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07940 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.33333) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53668 HOMO: -6.42733 LUMO: 2.15514 factor:1 | -1 (0.20939) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76806 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-0.02199) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26816 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (0.47791) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31747 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.42861) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.55127 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.19481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78527 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-2.03919) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31284 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-2.56677) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89027 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.14420) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48466 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-1.73859) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.30057 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (0.44550) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45317 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (0.29290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.16993 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (0.57615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58155 HOMO: -6.74570 LUMO: 2.20684 factor:1 | -1 (0.16452) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70887 HOMO: -6.30216 LUMO: 2.15242 factor:1 | -1 (0.03720) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99443 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.24836) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31718 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.57111) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16850 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.42243) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78147 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.03540) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45237 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.70630) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25528 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.50921) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95187 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.20580) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12994 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.38387) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47477 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.72869) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06118 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.31511) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03840 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.29233) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01955 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.27347) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72847 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (0.01761) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29882 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.55274) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10036 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.35429) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16472 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.41865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11563 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.36956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98648 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.24041) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92988 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.18381) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83516 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-0.08909) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31275 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.56668) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31528 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.56921) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45408 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.70801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72285 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.97678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67787 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-0.93180) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75069 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.00462) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69107 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.94500) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97592 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.22985) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03178 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-1.28571) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99094 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-1.24487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34278 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.59671) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57952 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.83345) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74415 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.99808) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88652 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-2.14045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42756 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-2.68149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51095 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.76488) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30855 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-1.56248) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14098 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-1.39491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42632 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-1.68025) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14283 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.39676) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84334 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-1.09727) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68729 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.94121) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83330 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.08723) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67580 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.92973) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75023 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.00415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79409 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.04802) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85010 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-3.10403) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11357 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-2.36750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03107 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-2.28499) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15540 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-2.40932) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81831 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-1.07224) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43172 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.68565) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36029 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.61422) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49398 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.74790) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65216 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.90608) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54767 HOMO: -6.69944 LUMO: 1.98915 factor:1 | -1 (0.19840) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65342 HOMO: -6.79468 LUMO: 1.96466 factor:1 | -1 (0.09265) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73347 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (0.01260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.38509 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (0.36099) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60625 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-0.86018) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61033 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.86426) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67082 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.92475) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81692 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-1.07085) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55313 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.80705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75998 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-3.01391) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15537 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-2.40930) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00538 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-2.25931) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26361 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-2.51754) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55653 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-1.81046) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04199 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-1.29592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15342 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.40735) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87164 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.12557) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90427 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.15820) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64652 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.90045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77937 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.03330) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75161 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-1.00554) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89956 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-1.15349) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91876 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-2.17269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78771 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-2.04164) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10209 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-2.35602) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86225 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-2.11618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12647 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-2.38040) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89297 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-2.14690) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96511 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-2.21903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50961 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-2.76353) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89757 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-2.15150) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65136 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.90529) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34252 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.59645) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55452 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-0.80845) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35237 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.60630) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40774 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-0.66167) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09609 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-0.35002) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23024 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.48417) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46649 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.72042) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84728 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-2.10121) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41250 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.66643) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62281 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.87674) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91808 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-2.17201) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50977 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-2.76370) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91811 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-2.17204) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96979 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-2.22371) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64311 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.89704) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85308 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-2.10700) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40730 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.66123) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66728 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.92121) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47111 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.72504) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35184 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.60577) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64619 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.90012) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35786 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.61178) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55147 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.80539) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77253 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-2.02646) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85368 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-2.10760) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71778 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.97171) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51334 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.76727) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42008 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.67401) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17756 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-3.43149) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64615 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-2.90008) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32721 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-2.58114) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53932 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.79325) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84845 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-2.10238) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81569 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-2.06962) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86260 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-2.11653) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76665 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-2.02058) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49712 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-1.75105) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68249 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-1.93642) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72004 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.97397) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25239 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.50631) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55481 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.80874) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45427 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.70819) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19720 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.45113) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10819 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.36212) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32210 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.57603) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94167 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.19560) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94738 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-0.20131) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84403 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.09796) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89495 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.14887) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65780 HOMO: -6.15249 LUMO: 0.32109 factor:1 | -1 (0.08827) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44811 HOMO: -6.84366 LUMO: 0.29116 factor:1 | -1 (0.29796) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68689 HOMO: -6.34297 LUMO: 0.19864 factor:1 | -1 (0.05918) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46358 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.71751) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20102 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.45495) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23280 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.48673) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44464 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.69857) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37417 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.62809) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36347 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.61740) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89470 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.14863) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.27959 HOMO: -6.57155 LUMO: -0.33470 factor:1 | -1 (0.46648) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56893 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (0.17715) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24702 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.50095) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98392 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.23785) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90569 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.15961) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21682 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-1.47075) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30640 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.56033) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91514 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.16906) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94191 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.19584) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89353 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.14746) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81938 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.07331) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.43439 HOMO: -6.70216 LUMO: 0.25034 factor:1 | -1 (0.31168) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58686 HOMO: -6.51713 LUMO: -0.78369 factor:1 | -1 (0.15921) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71747 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (0.02860) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45653 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.71046) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02823 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.28215) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30513 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.55906) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53977 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.79370) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16344 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.41737) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13900 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.39293) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84414 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.09807) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84417 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.09810) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07329 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.32722) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07457 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.32850) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17269 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-0.42662) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83104 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-2.08496) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67354 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.92746) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73775 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.99168) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34401 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.59793) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57087 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.82480) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49604 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.74996) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88105 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-2.13498) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75894 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-3.01287) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22472 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-3.47865) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10502 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-3.35895) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28936 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-2.54328) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52776 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-2.78168) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87577 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-2.12970) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24202 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.49595) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94345 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.19738) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51153 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.76546) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22958 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.48351) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75855 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.01248) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36322 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.61715) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46298 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.71691) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17566 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.42959) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84439 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.09831) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47071 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.72464) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09840 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.35233) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29422 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.54815) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11083 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.36476) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46292 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.71685) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11238 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.36631) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36621 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.62014) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84761 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-2.10154) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94184 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-2.19577) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20415 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-3.45808) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32370 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-2.57763) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69260 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-2.94653) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28187 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-2.53580) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65725 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-2.91118) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11826 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-1.37219) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35625 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-1.61018) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77672 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-2.03065) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.46588 HOMO: -6.78924 LUMO: 0.36735 factor:1 | -1 (0.28020) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68811 HOMO: -6.74298 LUMO: 0.51974 factor:1 | -1 (0.05796) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.57118 HOMO: -6.48992 LUMO: 1.44765 factor:1 | -1 (0.17489) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39613 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.34994) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32430 HOMO: -6.62325 LUMO: 1.57826 factor:1 | -1 (0.42178) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64542 HOMO: -6.19875 LUMO: 1.29798 factor:1 | -1 (0.10065) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78107 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.03499) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18880 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.44273) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32796 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.58189) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96012 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.21404) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17160 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.42553) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38470 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.63862) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22216 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.47609) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19212 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.44605) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10221 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.35614) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21966 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.47359) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98405 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-2.23797) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78282 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-2.03675) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92067 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-2.17460) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14888 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.40281) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44723 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.70116) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24712 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.50104) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46108 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.71501) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79042 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-1.04435) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69964 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.95357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13331 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-1.38724) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89910 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-1.15303) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06025 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-1.31417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74563 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.99956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47376 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.72769) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62514 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.87906) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74683 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.00075) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77706 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.03098) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42345 HOMO: -6.75114 LUMO: -0.62858 factor:1 | -1 (0.32262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56528 HOMO: -6.79468 LUMO: -0.64491 factor:1 | -1 (0.18079) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66844 HOMO: -6.84911 LUMO: -0.69661 factor:1 | -1 (0.07763) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79941 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.05333) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07710 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.33103) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12540 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.37933) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06074 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.31467) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28309 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.53702) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20965 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.46357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32538 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.57930) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21316 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.46708) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16461 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.41854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28597 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.53990) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59521 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (0.15086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54185 HOMO: -6.77564 LUMO: 1.97555 factor:1 | -1 (0.20422) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70166 HOMO: -6.40012 LUMO: 2.17691 factor:1 | -1 (0.04441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39744 HOMO: -6.80013 LUMO: 2.25582 factor:1 | -1 (0.34863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76183 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.01576) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44073 HOMO: -6.68856 LUMO: 1.85854 factor:1 | -1 (0.30534) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80055 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.05448) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38595 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54478 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.79871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65284 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.90677) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46429 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.71822) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34766 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.60159) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58650 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.84042) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43321 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.68714) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20018 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.45410) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16774 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-0.42167) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23188 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.48580) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06929 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-0.32322) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93535 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-0.18928) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37340 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.62733) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21234 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.46627) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06921 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.32314) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07160 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.32553) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19032 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.44425) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97231 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.22624) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.85829 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.11222) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28461 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.53854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79838 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-2.05231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93852 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-2.19245) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49340 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-1.74732) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79906 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-2.05299) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94413 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-2.19805) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79104 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.04497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47517 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.72910) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45939 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.71332) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65708 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.91101) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60364 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.85757) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77986 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.03379) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86196 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.11588) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76878 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-1.02271) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83864 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.09256) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97423 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-1.22816) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02166 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.27559) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08120 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.33513) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36243 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.61636) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62064 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.87457) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90489 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-2.15882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99093 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-2.24486) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71223 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.96616) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87455 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-2.12847) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43802 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.69195) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84554 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-2.09947) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94619 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-2.20012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68186 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-1.93579) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09810 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-1.35202) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01320 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.26713) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81006 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-2.06398) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72341 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-2.97733) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54951 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.80343) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57819 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.83212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70701 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.96093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97416 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.22809) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14105 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-0.39497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92229 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.17622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.82681 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.08074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11310 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.36703) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00678 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.26071) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10134 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.35527) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14242 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.39635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26722 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-1.52114) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12223 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.37616) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31198 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.56591) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36945 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.62338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75678 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-2.01070) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56591 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.81984) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62934 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-2.88326) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72121 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.97514) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72769 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.98161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52915 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.78308) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79049 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-2.04442) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41448 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-1.66841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60619 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.86012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73808 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-1.99201) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21688 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.47081) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33689 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.59081) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06586 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.31979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38336 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.63729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29825 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.55217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52549 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.77942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66944 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.92336) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78786 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-1.04179) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63806 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.89199) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68500 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.93893) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88881 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.14274) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96487 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.21880) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03320 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.28713) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30777 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-3.56170) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.99510 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-4.24903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69393 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.94785) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74127 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.99519) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01990 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-3.27383) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68823 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.94216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35632 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-3.61024) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.00011 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-4.25404) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69807 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-2.95200) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78564 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-3.03957) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00917 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.26310) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94400 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.19793) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16714 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-3.42107) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26848 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-3.52241) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12143 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-3.37535) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23071 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-3.48464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.89584 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-4.14976) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88278 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-3.13671) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61567 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-3.86960) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10344 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-3.35737) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93495 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-3.18888) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98140 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-3.23532) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57019 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.82412) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67901 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.93293) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60094 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.85486) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16516 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-3.41908) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.93097 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-4.18489) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23435 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-3.48828) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44019 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-2.69412) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55908 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-2.81300) | 1 | 1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76751 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.02143) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88400 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.13793) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82706 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-2.08099) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64570 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-1.89963) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51672 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.77064) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78132 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-2.03525) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61609 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-1.87002) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46001 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.71394) | 1 | 1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75036 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.00429) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88291 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.13684) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59300 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.84693) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87962 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.13354) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80876 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.06269) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78440 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-2.03832) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66491 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.91884) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58733 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.84126) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70731 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.96123) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63250 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.88643) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37511 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.62904) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83351 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-2.08744) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90130 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-2.15522) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87958 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-2.13351) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74333 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-1.99726) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84293 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-2.09685) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75259 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-2.00651) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66505 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-1.91897) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61767 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.87160) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79294 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.04687) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91065 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-3.16458) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00336 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-3.25728) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46402 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-3.71795) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92550 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-3.17943) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17536 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-3.42929) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25607 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-3.51000) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54906 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-2.80299) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79863 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-2.05255) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66652 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-1.92044) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67634 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.93027) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62164 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-1.87557) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78785 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.04178) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69354 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-1.94746) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41734 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.67127) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83294 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-2.08687) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63106 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.88499) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64499 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.89892) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50590 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-3.75982) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92518 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-3.17911) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76434 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-2.01827) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49718 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.75111) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40852 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-2.66244) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55230 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.80623) | 1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68690 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.94082) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41620 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.67013) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.58481 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-3.83874) | 1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86088 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-3.11481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11811 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-3.37203) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63696 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.89089) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80129 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.05522) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77854 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-2.03247) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72905 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.98298) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60270 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.85663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74946 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-2.00338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52890 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-2.78283) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41900 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-1.67293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70608 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-1.96001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07234 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-3.32627) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71252 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-2.96645) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.71850 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-3.97243) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64056 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.89449) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40236 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-0.65628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51360 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.76752) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53354 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.78747) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56973 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.82366) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25552 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.50945) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30597 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.55990) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86174 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.11567) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51297 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.76690) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08213 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.33606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35381 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.60774) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03011 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-3.28403) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93680 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-3.19073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68460 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-2.93853) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48609 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-0.74001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30793 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.56186) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37904 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.63296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58554 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.83947) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30691 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-2.56084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21326 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.46719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80792 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.06185) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44690 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.70083) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75946 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-3.01339) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76875 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-2.02268) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81988 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.07381) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42726 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.68119) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65843 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.91236) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60383 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.85776) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84530 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.09923) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61763 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.87155) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73811 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.99204) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74224 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.99617) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45824 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.71217) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59060 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.84452) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67558 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.92950) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54738 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.80131) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16812 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.42205) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38570 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.63963) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69524 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.05083) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97272 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.22664) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.47358 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.27249) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53121 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.21486) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07887 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.33280) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03310 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.28703) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87307 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.12700) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21237 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.46629) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14755 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.40148) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13193 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.38586) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16363 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.41756) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33683 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.59076) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00439 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.25832) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37128 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.62521) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98091 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.23483) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01707 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.27100) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11971 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.37364) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92297 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.17690) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10371 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.35764) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72355 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.97748) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51685 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.77078) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64801 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.90194) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.37167 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.37440) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60490 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.14117) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.30585 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.44023) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68213 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.06395) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32721 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.41886) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42147 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.32460) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63252 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.11355) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23591 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.51016) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76594 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.01986) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68789 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.05818) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29493 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.54885) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19337 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.44730) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38682 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.64075) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54014 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.20594) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54416 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.20191) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33483 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.41125) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.28756 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.45851) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32960 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.41647) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89426 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.14818) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77515 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.02908) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90125 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.15518) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85088 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.10481) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36535 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.61928) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43408 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.68801) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35247 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.60640) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38771 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.64164) | 1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59022 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.84415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66625 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.92018) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37111 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.62504) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56782 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.82175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73354 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.98747) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75473 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.00866) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31461 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.56854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62823 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.88216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03838 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-3.29231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24283 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.49675) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35902 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.61295) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89969 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.15362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.08333) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11681 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.37074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94109 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.19502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01853 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.27246) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22923 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.48316) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03543 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.28936) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19685 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.45078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86111 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.11504) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97956 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.23349) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58541 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.83934) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71817 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.97210) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51945 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.77337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78244 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.03637) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39003 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.64396) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58059 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.83452) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73314 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.98707) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90538 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.15931) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56161 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.81553) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89027 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.14420) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98426 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.23819) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60739 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.86132) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46244 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.71637) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24260 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.49653) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19013 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.44406) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91035 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.16428) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29465 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.54858) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19612 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.45005) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23580 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.51027) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45306 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.29301) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.92529 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.82078) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50726 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.23881) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.14592 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.60015) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27514 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.52907) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42619 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.68012) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41833 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.67226) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23647 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.49039) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28670 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.54063) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81193 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.06586) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82687 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.08080) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76018 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.01411) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61528 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.86920) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25846 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.51239) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18592 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.43984) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98714 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.24107) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27269 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.52662) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18962 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.44355) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20430 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.45823) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07660 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.33053) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18017 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.43409) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05154 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.30547) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82435 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.07828) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10378 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.35771) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62722 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.88115) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35078 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.60471) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00020 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-3.25413) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55448 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.80841) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14350 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.39743) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52465 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.77858) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11960 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.37353) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76485 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.01878) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35713 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.61106) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06077 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.31470) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02869 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.28262) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02420 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.27813) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19615 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.45008) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90741 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.16134) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20426 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.45819) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51654 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.77046) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34478 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.59870) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43939 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.69332) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24703 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.50096) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38679 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.64072) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46328 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.71721) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42320 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.67713) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48483 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.73876) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57686 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.83079) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67463 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.92856) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41011 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.66404) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02003 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.27396) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54375 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.79767) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39663 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.65056) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53106 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-1.78499) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09778 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-3.35171) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23673 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.49066) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29804 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-2.55197) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36979 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-2.62372) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18689 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.44082) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26025 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.51418) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30904 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-1.56297) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40798 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.66191) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67691 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.93084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82897 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.08290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89095 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.14488) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52387 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.77780) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59985 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.85378) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45383 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.70776) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63947 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.89340) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41084 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.66477) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65158 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.90550) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01361 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.26753) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38379 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.63772) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62774 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.88167) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29209 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.54601) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09522 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-3.34915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71595 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.96988) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92382 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-3.17775) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03106 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-3.28499) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72836 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-2.98229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81579 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-3.06972) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82648 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-3.08041) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45654 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.71047) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66970 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.92363) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31133 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.56525) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27922 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.53314) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50883 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.76275) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30376 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.55769) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45489 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.70882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65672 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.91065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33323 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.58716) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31622 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.57015) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61484 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.86877) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05116 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.30509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31598 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.56991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18047 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.43439) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27532 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.52925) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53016 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.78409) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43669 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.69062) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34920 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.60313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52001 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.77394) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22106 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-2.47498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35820 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-2.61213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45674 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-1.71067) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74241 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.99634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.31234 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-3.56627) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54947 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-2.80340) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80433 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-3.05826) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34317 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-3.59710) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23024 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-3.48417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.96321 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-4.21714) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98836 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-3.24229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71612 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.97005) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70262 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-2.95654) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67359 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.92752) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82042 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-2.07435) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64945 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-2.90337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45175 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-2.70568) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21629 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-3.47021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30440 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-2.55833) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45736 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.71129) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21895 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-3.47288) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.94332 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-4.19725) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02515 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-3.27908) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.64372 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-3.89765) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.48952 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-3.74344) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62547 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-2.87940) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83231 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-3.08623) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48094 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.73487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64146 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.89539) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43112 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.68505) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56312 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.81705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65969 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.91362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43025 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.68418) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56813 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.82206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37098 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-3.62491) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97081 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-3.22474) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64467 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.89860) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46394 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.71786) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59738 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-0.85131) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86446 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-1.11839) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43992 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-2.69385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26313 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-2.51705) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45113 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-2.70506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58105 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.83498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96710 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-1.22103) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79619 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.05011) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55199 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.80592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58391 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.83784) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21498 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.46891) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48894 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-0.74287) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57399 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-2.82792) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50824 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.76216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50892 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-0.76284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14379 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.39772) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24494 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.49887) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91163 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.16555) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37060 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.62453) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39371 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.35236) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.90799 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.83808) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.16614 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (0.57993) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79590 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.04982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53894 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-2.79287) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91188 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-2.16581) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44980 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.70373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68992 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-1.94385) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40173 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.65566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93740 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-0.19132) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70079 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.04528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15285 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.40678) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13013 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.38406) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44960 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-0.70352) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72567 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.97960) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56680 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-2.82073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69803 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-1.95195) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90527 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-2.15920) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61460 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-1.86852) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84331 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-2.09724) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10588 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-1.35981) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46874 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-1.72267) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78597 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-2.03990) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51238 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-2.76631) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45207 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-0.70600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41759 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.67152) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12175 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.37568) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26298 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.51691) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75861 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-1.01254) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71715 HOMO: -6.16882 LUMO: 1.94017 factor:1 | -1 (0.02893) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09530 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.34923) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44685 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.70077) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46077 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.71470) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31824 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.57217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37489 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.62882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45487 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.70879) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73522 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.98915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81667 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-2.07060) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55843 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.81236) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88886 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-2.14279) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41846 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-1.67238) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57476 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.82869) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62249 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.87642) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59650 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-1.85043) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.94288 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (1.80319) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.22708 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (1.51899) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.92860 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (1.81748) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66103 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-0.91496) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94043 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-1.19436) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11736 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.37129) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11363 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.36756) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15211 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.40604) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53584 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.78977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61226 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.86618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54896 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-1.80289) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60251 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.85644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72919 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-0.98312) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59314 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-0.84706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95287 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-1.20680) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83357 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.08750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95505 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-1.20897) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23552 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-0.48945) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02654 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-0.28047) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64897 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-0.90290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17696 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.43089) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64933 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-0.90325) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01680 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-0.27073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80828 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-0.06221) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99402 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.24795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00287 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-0.25679) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64866 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-1.90259) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53173 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-2.78566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77642 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-2.03035) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49457 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-1.74849) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63435 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-1.88828) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32493 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-1.57886) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36768 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-1.62161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35018 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-1.60411) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44523 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.69916) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83999 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.09392) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82551 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-2.07944) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82584 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-2.07977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98279 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-2.23672) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81201 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-2.06594) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53862 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.79255) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75931 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-2.01323) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67443 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.92836) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75803 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-2.01196) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42351 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-2.67744) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33613 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-2.59006) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22609 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-2.48002) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51810 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-2.77202) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33903 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.59295) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48602 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-1.73995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56270 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-1.81663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48717 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-1.74109) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60886 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.86279) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08035 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.33428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83804 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.09197) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03576 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.28968) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72766 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.98159) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65844 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.91237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09385 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-1.34778) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83605 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-1.08998) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11505 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-1.36898) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78957 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-1.04350) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95491 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-1.20884) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03891 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-1.29284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34295 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-3.59688) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94325 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-3.19717) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56158 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-2.81551) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74044 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-2.99437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51131 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.76524) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81760 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-1.07153) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.59349 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-3.84742) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82422 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-3.07815) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99566 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-3.24958) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41203 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-1.66596) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57125 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-1.82518) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22310 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-2.47703) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35826 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-2.61218) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45876 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-1.71268) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68031 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-1.93424) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61282 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-2.86675) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95348 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-3.20741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34796 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-3.60189) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42385 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-3.67778) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84534 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-3.09927) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75903 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-3.01295) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98698 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-3.24090) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15959 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.41352) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27247 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.52640) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23886 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.49279) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20860 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.46253) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82974 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.08367) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19268 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.44661) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17238 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.42631) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00599 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.25991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69742 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-2.95135) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52408 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-2.77801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74185 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-2.99578) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45253 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-0.70646) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40832 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-0.66224) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59164 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-0.84557) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37985 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-0.63378) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29835 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-0.55228) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52094 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.77487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82087 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-1.07480) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65507 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.90900) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44440 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.69833) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21316 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.46708) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31046 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-0.56439) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39501 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.64894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69745 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-2.95137) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53812 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-2.79205) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74545 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-2.99938) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85878 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-3.11271) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74977 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-3.00370) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12069 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-3.37462) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81079 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-2.06472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89425 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-2.14818) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13606 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-1.38998) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77004 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.02396) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77349 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.02742) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18052 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.43445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98541 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.23934) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96563 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.21956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13197 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.38590) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92421 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-2.17814) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53707 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-1.79100) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75743 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-2.01136) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44150 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-2.69542) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62004 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.87397) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67694 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.93087) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23962 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.49355) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71327 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-0.96720) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35305 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.60698) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35906 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.61299) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70334 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.95727) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78111 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-1.03504) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40750 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.66143) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38268 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.63661) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73393 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.98785) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20902 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.46295) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17296 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.42689) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59455 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.84848) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55673 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.81065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95599 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-2.20992) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57604 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-1.82997) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21667 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.47059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57482 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.82875) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13357 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-2.38750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23045 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-1.48438) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60866 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-1.86259) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91555 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-2.16948) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54493 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.79886) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73365 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.98757) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55679 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-2.81072) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59528 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.84920) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71756 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.97149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33249 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-2.58642) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23287 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.48680) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96649 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-2.22042) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68482 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-2.93875) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52785 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.78177) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28849 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-2.54241) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46395 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-2.71787) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31783 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.57176) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68322 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.93715) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59441 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.84833) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37965 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.63358) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37701 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.63094) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12861 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.38254) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97816 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.23209) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23106 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.48499) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21813 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.47205) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35345 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-1.60738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11421 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-1.36813) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02844 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-1.28236) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49048 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-1.74441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56815 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-1.82207) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38281 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-1.63674) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35149 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-1.60542) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43402 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-1.68795) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69394 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-1.94787) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42738 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-1.68131) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28673 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.54065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63441 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-1.88833) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46700 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-1.72093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41114 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-1.66506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22887 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-1.48280) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01755 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-1.27148) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25813 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-1.51206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89316 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-2.14709) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20126 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-1.45518) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02169 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-1.27562) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24732 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-1.50125) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54249 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.79642) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31509 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.56902) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38562 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.63955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52258 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-0.77650) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18456 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.43848) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36619 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-0.62012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74636 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-1.00029) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43876 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-0.69269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52524 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.77917) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37542 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.62934) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27781 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.53174) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21454 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.46847) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41566 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.66959) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21615 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.47008) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11196 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.36588) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03832 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.29225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39093 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-0.64486) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23941 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.49334) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81075 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.06468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67497 HOMO: -6.09807 LUMO: 0.20136 factor:1 | -1 (0.07110) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92752 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.18145) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80585 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.05977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09423 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-1.34816) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84196 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-1.09588) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08052 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-1.33445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27754 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-0.53147) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54454 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.79846) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65590 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-1.90983) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33763 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-2.59156) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61813 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-1.87206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49059 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-1.74452) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71925 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.97318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54789 HOMO: -6.35658 LUMO: 0.07891 factor:1 | -1 (0.19818) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50756 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.23851) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.41333 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.33274) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.47124 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (0.27483) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60993 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (0.13614) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70517 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (0.04090) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35712 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-1.61105) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60461 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-1.85854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22239 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-2.47632) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69348 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-1.94741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61819 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-1.87212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51517 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-1.76909) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76105 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.01498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35984 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-1.61377) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61223 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-1.86616) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75728 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.01121) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01364 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.26757) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.04576 HOMO: -6.75931 LUMO: 1.13744 factor:1 | -1 (0.70031) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25670 HOMO: -6.15794 LUMO: 1.12383 factor:1 | -1 (0.48937) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.01985 HOMO: -6.59604 LUMO: 1.19458 factor:1 | -1 (0.72622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05395 HOMO: -7.09401 LUMO: 0.60137 factor:1 | -1 (0.69212) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24375 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (0.50232) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.36125 HOMO: -6.72665 LUMO: -2.47624 factor:1 | -1 (0.38482) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79875 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.05268) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67391 HOMO: -6.94162 LUMO: 0.28300 factor:1 | -1 (0.07216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72743 HOMO: -6.65591 LUMO: 0.57144 factor:1 | -1 (0.01864) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88909 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.14302) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01829 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.27222) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.75534 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-4.00927) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91587 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-3.16980) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15220 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-3.40613) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25503 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.50896) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50375 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.75767) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34447 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.59840) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57119 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-1.82512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68926 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-2.94318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91176 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-3.16569) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33269 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-1.58661) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56270 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.81663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.77213 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-4.02606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93225 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-3.18618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18037 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-3.43429) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32146 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.57538) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23781 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.49174) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54998 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.80391) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86931 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.12324) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64101 HOMO: -6.52257 LUMO: -0.59865 factor:1 | -1 (0.10506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84420 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.09812) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.12818 HOMO: -6.79740 LUMO: -0.75376 factor:1 | -1 (0.61789) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.88116 HOMO: -5.89127 LUMO: 0.22313 factor:1 | -1 (0.86491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.07923 HOMO: -6.34842 LUMO: 0.11429 factor:1 | -1 (0.66684) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26647 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (0.47960) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.17373 HOMO: -6.50080 LUMO: 1.74153 factor:1 | -1 (0.57234) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.34949 HOMO: -6.33481 LUMO: 1.68438 factor:1 | -1 (0.39658) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13975 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-2.39368) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63190 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.88583) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35078 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-1.60471) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58156 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-1.83549) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51482 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.76875) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89192 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.14584) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60171 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.85563) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82046 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.07439) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42959 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-0.68352) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16486 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-0.41878) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35297 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-0.60690) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44967 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.70360) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57694 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.83086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39582 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.64974) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60371 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.85764) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21619 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.47012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22243 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.47635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37051 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.62444) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55431 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-2.80824) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56729 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-2.82122) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73826 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-2.99219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69529 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-3.94922) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87135 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-3.12528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77386 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-3.02778) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90629 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-3.16022) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19332 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.44725) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43738 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.69131) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52598 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-0.77991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32840 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-0.58232) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21019 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-0.46412) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24815 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-0.50208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43096 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-0.68488) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76321 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.01713) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50742 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-0.76135) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11694 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-0.37086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38595 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83576 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-3.08969) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73347 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-2.98740) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95087 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-3.20479) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21569 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-0.46961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07479 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-0.32871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15536 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-0.40929) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26412 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-0.51805) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41634 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.67027) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89392 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-2.14785) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65209 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.90602) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71340 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.96733) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29933 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-0.55326) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34094 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-0.59487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51708 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-0.77101) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37116 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.62509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39111 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.64504) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59462 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.84855) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95025 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-2.20418) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60400 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-2.85793) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71667 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.97059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74075 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.99468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32109 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-2.57501) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30531 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-1.55924) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38599 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.63992) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54962 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-1.80354) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04688 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-1.30081) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18267 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.43660) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03339 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.28732) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23734 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.49127) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20219 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-0.45612) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14728 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-0.40120) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34287 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.59680) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29838 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.55231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25016 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-0.50409) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17231 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-0.42624) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37501 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-0.62894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26208 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-0.51601) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28518 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.53910) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47204 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.72596) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32564 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-1.57957) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53849 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-1.79241) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14560 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-2.39953) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25581 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-1.50974) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42806 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-1.68199) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28436 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-1.53829) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49212 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-1.74605) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01612 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-2.56331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91712 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-2.46432) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97000 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-2.51719) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02096 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-2.56816) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04543 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-2.59262) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97174 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-2.51893) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07544 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-2.62263) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18592 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-2.73311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08303 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-2.63023) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91078 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-2.45798) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90485 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-2.45205) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95266 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-2.49986) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68667 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-2.23386) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85895 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-2.40614) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41425 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-2.96144) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82820 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-2.37539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91601 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-2.46320) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59581 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-2.14301) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70166 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-2.24886) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80920 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-2.35640) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52419 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-2.07139) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06336 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-2.61055) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13672 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-2.68391) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93560 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-2.48279) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17743 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-2.72462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23737 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-2.78457) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03016 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-2.57735) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16227 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-2.70946) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96151 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-2.50870) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08521 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-2.63240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80645 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-2.35365) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87835 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-2.42554) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88708 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-2.43428) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67083 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-2.21803) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75225 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-2.29944) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19084 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-2.73804) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24529 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-2.79249) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06251 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-2.60971) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93522 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-2.48241) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72267 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-2.26986) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89794 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-2.44513) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77538 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-2.32257) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03726 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-2.58446) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88768 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-2.43487) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05435 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-2.60154) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10826 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-2.65545) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89979 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-2.44698) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75704 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-2.30423) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60637 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-2.15356) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95576 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-2.50296) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97236 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.51956) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92537 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-2.47256) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65957 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-2.20676) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95835 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-2.50554) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84371 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-2.39090) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70349 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-2.25068) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97595 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-2.52315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96929 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-2.51648) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96194 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-2.50913) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66855 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-2.21574) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08709 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-2.63428) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04352 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-2.59071) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78689 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-2.33408) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98001 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-2.52720) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89103 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-2.43822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72213 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-2.26932) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85097 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-2.39817) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78890 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-2.33610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59976 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.14695) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77916 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-2.32636) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65682 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-2.20401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61837 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-2.16556) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80145 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-2.34864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60427 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-2.15147) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60183 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-2.14902) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50438 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-2.05158) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68906 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-2.23626) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90373 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-0.45092) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70269 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.24988) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94452 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.49171) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71395 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.26115) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64203 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.18923) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85377 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.40096) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21268 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.75988) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98487 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.53206) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11597 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.66317) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30354 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.85074) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14215 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.68935) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26479 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.81199) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17143 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-0.71863) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76195 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.30915) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18491 HOMO: -6.53345 LUMO: -0.84627 factor:1 | -1 (0.26790) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10687 HOMO: -6.60148 LUMO: -0.63130 factor:1 | -1 (0.34594) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98137 HOMO: -6.36202 LUMO: -0.60137 factor:1 | -1 (0.47144) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15664 HOMO: -6.28855 LUMO: -0.52790 factor:1 | -1 (0.29617) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04485 HOMO: -7.07224 LUMO: 0.41906 factor:1 | -1 (0.40795) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52705 HOMO: -6.36202 LUMO: -0.24218 factor:1 | -1 (0.92576) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11998 HOMO: -6.43549 LUMO: 0.14150 factor:1 | -1 (0.33282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03892 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.41389) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37457 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (0.07823) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79277 HOMO: -6.33753 LUMO: -0.02993 factor:1 | -1 (0.66004) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38722 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-0.93441) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24130 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (1.21151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23052 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (1.22228) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96964 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (0.48317) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78028 HOMO: -6.59604 LUMO: -0.79729 factor:1 | -1 (0.67253) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20260 HOMO: -7.09401 LUMO: 0.31837 factor:1 | -1 (0.25021) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05114 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.40167) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01862 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.43418) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39062 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-0.93781) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48670 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.03390) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33558 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.11723) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21332 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.23949) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07669 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (0.37612) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55028 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-0.09747) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65953 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-0.20672) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95905 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-0.50624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63357 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-0.18077) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75553 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-0.30273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68193 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-0.22912) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09793 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.64513) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65732 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-1.20451) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50572 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-1.05292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59655 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.14375) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68894 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.23613) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98432 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.53151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44801 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.99520) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39987 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.94707) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58583 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.13303) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73171 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.27891) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73740 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.28460) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59851 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.14571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52439 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.07158) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71299 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-1.26019) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73014 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.27733) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85417 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-0.40137) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01420 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-0.56140) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84903 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-0.39622) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95545 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.50265) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83762 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.38481) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95629 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-1.50348) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58156 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.12876) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62439 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.17159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84875 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.39594) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92805 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-0.47525) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87023 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.41742) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03932 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-0.58651) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72897 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.27617) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76944 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-0.31663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77874 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.32594) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42619 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.02661) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30897 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.14384) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95348 HOMO: -6.64230 LUMO: 2.23405 factor:1 | -1 (0.49933) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03849 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.41432) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13155 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.32126) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99470 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (0.45810) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26456 HOMO: -6.56611 LUMO: 1.60003 factor:1 | -1 (0.18825) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14328 HOMO: -6.70489 LUMO: 1.78779 factor:1 | -1 (0.30953) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28286 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-0.83006) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01102 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-0.55821) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14672 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-0.69392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33696 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-0.88415) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03573 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-0.58292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12882 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.67601) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33221 HOMO: -6.13345 LUMO: 2.07351 factor:1 | -1 (0.12060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27093 HOMO: -6.46270 LUMO: -0.37552 factor:1 | -1 (0.18188) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27405 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.17875) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05759 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (0.39522) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87992 HOMO: -6.51168 LUMO: 1.92112 factor:1 | -1 (0.57288) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84039 HOMO: -6.71305 LUMO: 1.91024 factor:1 | -1 (0.61242) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09557 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-0.64276) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34425 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-0.89145) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11913 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.66633) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11573 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.66292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71860 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-1.26579) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41457 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.96176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45359 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.00078) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49400 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.04120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10869 HOMO: -6.92258 LUMO: 1.87214 factor:1 | -1 (0.34412) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98983 HOMO: -5.85861 LUMO: 2.11705 factor:1 | -1 (0.46297) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32700 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-0.87419) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02520 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.57239) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41693 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.96413) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22196 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-0.76916) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14452 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.69171) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09815 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.64535) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93102 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.47821) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88196 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-0.42915) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40368 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.95087) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62976 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.17696) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77380 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-2.32100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90311 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-2.45030) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86714 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-2.41433) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72607 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-2.27327) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97869 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-0.52589) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23745 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.78464) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49680 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.04399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83981 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.38700) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93431 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.48151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13089 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-0.67808) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88890 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.43609) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83812 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.38531) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44752 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.99471) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85079 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-1.39798) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15997 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.70716) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23039 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-1.77758) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17349 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-1.72068) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94483 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-1.49203) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21387 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.76107) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00347 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.55067) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90652 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-1.45371) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91985 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-1.46705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80448 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.35167) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80339 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-1.35058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60439 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-1.15159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01259 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.55978) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03161 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.57880) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96162 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-1.50882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81800 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.36520) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98383 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.53102) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98502 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.53222) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96124 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.50844) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94173 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.48893) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18500 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.73220) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88600 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.43320) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29540 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.84259) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97085 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.51804) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23869 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.78588) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96166 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-0.50885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68582 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-0.23301) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17829 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-0.72548) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14743 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.69463) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01660 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-0.56379) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11924 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.66643) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57484 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.12203) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38213 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.92932) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45073 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.99792) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47525 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.02244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57408 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.12127) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39685 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-0.94404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72635 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.27355) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00549 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.55268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77030 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.31749) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73231 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.27951) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94336 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.49056) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03428 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.58147) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95885 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.50604) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92187 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.46906) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08694 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-0.63413) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98833 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-0.53552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12738 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-0.67457) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19211 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.73931) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10833 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.65552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04128 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.58847) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91235 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.45955) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88792 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.43511) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88337 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-0.43057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32357 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-0.87076) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02180 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-0.56899) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90326 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.45046) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06109 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.60828) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96179 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-0.50899) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04996 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-0.59715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38738 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-0.93458) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38521 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.06759) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17035 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (0.28245) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08298 HOMO: -6.65318 LUMO: -0.73199 factor:1 | -1 (0.36983) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09351 HOMO: -6.51441 LUMO: -0.44899 factor:1 | -1 (0.35930) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93916 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (0.51364) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42097 HOMO: -6.96884 LUMO: 0.19864 factor:1 | -1 (0.03184) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30007 HOMO: -6.89809 LUMO: 0.34558 factor:1 | -1 (0.15274) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15900 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.70619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04874 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-0.59593) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85687 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-0.40406) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30145 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.84864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41258 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.95977) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19829 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.74548) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89562 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.44281) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17535 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.72254) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89409 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.44129) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73638 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-0.28357) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61692 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.16411) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20678 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.75397) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59620 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.14340) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34752 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-0.89471) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60959 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.15678) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04680 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.59400) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12400 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.67120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27086 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.81806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97946 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.52665) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11004 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-0.65724) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12446 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.67166) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88551 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-1.43271) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10900 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.65619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94960 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.49679) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12639 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-1.67358) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78589 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.33309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95221 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.49940) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62524 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.17243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67443 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-1.22163) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64668 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.19387) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84782 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.39502) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79196 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.33915) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13573 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.68292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90732 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.45451) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99325 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-0.54045) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24572 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-0.79291) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30980 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-0.85700) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36319 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-0.91038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87071 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.41790) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78905 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.33624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72254 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.26974) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07673 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.62392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63321 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.18040) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58042 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.12761) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69609 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.24329) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98478 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.53197) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85495 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-1.40215) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95052 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-1.49771) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84073 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.38793) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31952 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.13328) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26948 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.18332) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17901 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (0.27380) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12477 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.32803) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32655 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (0.12626) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91390 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-0.46110) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76884 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-0.31603) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77526 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-0.32245) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13524 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-0.68243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81681 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.36401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89733 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-0.44453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79986 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.34705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06621 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-0.61340) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01722 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.56442) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95031 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.49751) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96601 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.51321) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95154 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-0.49873) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03344 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.58064) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17734 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.72453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31285 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.86004) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22139 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.76859) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28896 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-0.83615) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10253 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.64973) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02679 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.57399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84385 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.39105) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02952 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.57671) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27507 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.82226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04784 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.59503) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18784 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.73503) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17774 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.72494) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03684 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-1.58403) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87879 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.42599) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01615 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.56335) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32341 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.87060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54125 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.91155) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42895 HOMO: -6.88448 LUMO: 2.24494 factor:1 | -1 (1.02386) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44882 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.99602) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32825 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-0.87544) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26835 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (1.18446) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.15885 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (1.29396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91473 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.53808) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88978 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.56303) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46295 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-1.01014) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31905 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-0.86625) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77719 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-0.32439) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80190 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-0.34909) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96661 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-0.51381) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89072 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-0.43791) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98073 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.52793) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39261 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-0.93980) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61337 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.16057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54322 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.09041) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47988 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.02708) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61953 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-0.16672) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40981 HOMO: -6.94162 LUMO: 2.21773 factor:1 | -1 (0.04299) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21290 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.76010) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76782 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.31502) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76720 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.31439) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76956 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.31676) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84143 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.38862) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54341 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.09061) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70445 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.25164) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79629 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.34348) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68317 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.23036) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22166 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.76886) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29584 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.84304) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26904 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-0.81623) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28395 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-0.83114) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03510 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.58230) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23935 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.78655) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19674 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-0.74393) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25032 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-0.79751) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36921 HOMO: -6.41100 LUMO: 1.80956 factor:1 | -1 (0.08359) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49711 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.04430) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27190 HOMO: -6.78380 LUMO: -0.76192 factor:1 | -1 (0.18090) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54524 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.09244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41142 HOMO: -6.57155 LUMO: 1.89119 factor:1 | -1 (0.04139) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58878 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.13598) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09236 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.63955) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30531 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.85251) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98068 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-0.52787) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15029 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.69748) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92895 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.47614) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18980 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-0.73699) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74117 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-0.28836) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47244 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.01964) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92003 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-0.46722) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13761 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-0.68480) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14471 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-0.69190) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15094 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-0.69814) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26972 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-0.81691) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31584 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.86304) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16841 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-0.71561) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99826 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-0.54545) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10082 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.64801) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02454 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.57174) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17184 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.71903) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13189 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-0.67909) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19837 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-0.74556) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08670 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.63389) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41914 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.96633) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08626 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-0.63345) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01181 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-0.55900) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25323 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.80042) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40983 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.95702) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37407 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-0.92127) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38975 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-0.93694) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18271 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.27010) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31103 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.14177) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70244 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.24964) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61689 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-0.16408) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80772 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.35492) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89709 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-0.44428) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19072 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-0.73792) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02808 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-0.57528) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08631 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-0.63351) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98160 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-0.52880) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35315 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-0.90034) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39419 HOMO: -6.77836 LUMO: 0.25851 factor:1 | -1 (0.05861) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40717 HOMO: -5.70623 LUMO: 0.73471 factor:1 | -1 (0.04563) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33806 HOMO: -5.58378 LUMO: 0.89253 factor:1 | -1 (0.11475) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48923 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.03643) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50472 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-1.05191) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48323 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-0.03042) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64968 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.19687) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70081 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-0.24800) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77880 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-0.32599) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96612 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.51332) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36946 HOMO: -4.72934 LUMO: 1.00410 factor:1 | -1 (0.08335) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30200 HOMO: -4.56335 LUMO: 1.56738 factor:1 | -1 (0.15081) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16499 HOMO: -5.48854 LUMO: 0.33198 factor:1 | -1 (0.28781) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51977 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.06697) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24200 HOMO: -4.60145 LUMO: 1.74697 factor:1 | -1 (0.21081) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26216 HOMO: -5.60010 LUMO: 0.74831 factor:1 | -1 (0.19064) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40845 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.04435) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43354 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.01927) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72138 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.26858) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63281 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-0.18000) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96264 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.50983) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96457 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-0.51176) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22240 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.76959) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33161 HOMO: -5.27629 LUMO: 0.57960 factor:1 | -1 (0.12120) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25248 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (0.20033) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21563 HOMO: -5.08853 LUMO: 0.89253 factor:1 | -1 (0.23717) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30137 HOMO: -6.42461 LUMO: 0.04354 factor:1 | -1 (0.15143) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27509 HOMO: -6.42733 LUMO: -0.00544 factor:1 | -1 (0.17772) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29063 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (0.16218) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36162 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (0.09119) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42021 HOMO: -4.44362 LUMO: 1.99187 factor:1 | -1 (0.03260) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07494 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.62213) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23078 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-0.77797) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85804 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.40523) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06621 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.61340) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41723 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.96443) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28381 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-0.83101) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43310 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-0.98029) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81172 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.35892) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81689 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.36409) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56805 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.11524) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68252 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.22972) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85243 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-0.39963) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90310 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.45029) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04833 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.59552) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80647 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.35367) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94389 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.49108) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89788 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.44507) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67768 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.22487) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75605 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.30324) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55806 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-0.10525) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47811 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.02531) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46573 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.01293) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44559 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (0.00721) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25163 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.20117) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23008 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (0.22273) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48665 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.03384) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52145 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.06865) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36850 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-0.91569) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52308 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-1.07028) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88098 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-0.42817) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75110 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.29829) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63602 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-0.18321) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71096 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.25815) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50135 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.04855) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.20881 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (1.24400) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72946 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-0.27666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.61302 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (1.83979) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.68662 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (1.76618) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.62869 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (1.82412) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.54417 HOMO: -5.74160 LUMO: 0.14694 factor:1 | -1 (1.90863) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.70287 HOMO: -4.78376 LUMO: 0.92791 factor:1 | -1 (1.74994) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.40363 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (2.04918) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27002 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.81721) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81006 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.35725) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47536 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-1.02255) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72029 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-1.26748) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22781 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.77501) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12071 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-0.66790) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16762 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-0.71482) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52066 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.06786) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13638 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.68358) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58198 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.12917) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86013 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.40733) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38110 HOMO: -5.00690 LUMO: 1.14288 factor:1 | -1 (0.07170) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56549 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-0.11268) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72481 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.27201) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04346 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.59065) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95823 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-0.50542) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79589 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-0.34308) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92215 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.46934) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24370 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.79090) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33342 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.88061) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35323 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.90042) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24128 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-0.78848) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25750 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-0.80470) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16613 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-0.71332) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36186 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-0.90905) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34602 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.89321) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21021 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-0.75740) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18044 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-0.72763) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07755 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.62475) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19998 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.74717) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04759 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.59479) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14819 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-0.69539) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26166 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.80885) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50104 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.04824) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27377 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.82097) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18871 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.73590) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69819 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-1.24538) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58692 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.13412) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63462 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-1.18182) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42580 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.97300) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07320 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.62039) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91597 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.46317) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94944 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.49664) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03595 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.58314) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90166 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.44885) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71409 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.26128) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65510 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.20229) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24006 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.78725) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98999 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.53718) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20259 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.74978) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13241 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.67960) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20395 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.75114) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04411 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.59130) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21445 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.76165) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26985 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-1.81704) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53766 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-2.08485) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17197 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.71916) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13077 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-1.67796) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21774 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.76493) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56260 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-1.10979) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68657 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-1.23376) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71297 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-1.26016) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60668 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.15387) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73188 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-1.27907) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78472 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.33192) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50420 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-1.05139) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30879 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.85599) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34300 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.89019) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31312 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.86032) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14430 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.69150) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03464 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.58183) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40898 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.95617) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23262 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-1.77982) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21208 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-1.75927) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86543 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-1.41262) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31529 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-1.86248) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21115 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.75835) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76847 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-2.31566) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82719 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-2.37438) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57908 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-2.12627) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55807 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-2.10526) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76692 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-2.31411) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39050 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.93770) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42313 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.97032) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33404 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.88123) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18476 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.73195) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34862 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-1.89582) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43971 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.98690) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17667 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.72387) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95670 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.50389) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10192 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.64912) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59533 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.14252) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85947 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.40667) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48102 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-1.02821) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98644 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-1.53363) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65530 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-1.20250) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03411 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-1.58131) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91735 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-1.46454) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13942 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.68662) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84693 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.39412) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04837 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-1.59557) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85433 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.40152) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83694 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.38413) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06699 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-1.61418) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64779 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-1.19499) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60540 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-1.15259) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57857 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-1.12576) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45258 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-0.99977) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64072 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-1.18791) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69454 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-1.24174) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91637 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.46356) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31665 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-1.86384) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05591 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-1.60310) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13825 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-1.68545) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11515 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-1.66234) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24185 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-1.78904) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07727 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-1.62447) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07365 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-1.62085) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34261 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-1.88980) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46022 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-2.00741) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30577 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-1.85296) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20432 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.75152) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35192 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.89911) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55562 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-2.10281) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48103 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-2.02823) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44444 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.99164) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91276 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.45995) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49156 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.03875) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44143 HOMO: -6.57971 LUMO: 0.12789 factor:1 | -1 (0.01137) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76982 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.31701) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57196 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-1.11915) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56877 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-1.11597) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52608 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-1.07327) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45623 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-1.00342) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63653 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-1.18372) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29221 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-1.83941) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26838 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.81557) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08073 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.62792) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45818 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-2.00537) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91865 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-2.46584) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78273 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-2.32992) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93253 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-2.47972) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75732 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.30451) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60303 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.15023) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61753 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-2.16472) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52464 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-1.07183) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57336 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-2.12056) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67109 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-1.21828) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55159 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-2.09879) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36479 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.91198) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50568 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-3.05287) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02461 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-2.57180) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02488 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-2.57207) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88278 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-2.42998) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18638 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-2.73357) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.90686 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-3.45405) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25825 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-2.80544) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76979 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-3.31699) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14175 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-2.68895) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06167 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-2.60886) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99634 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-2.54353) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.87037 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-3.41756) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.99290 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-3.54009) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21944 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-2.76664) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07008 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-2.61727) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35219 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-1.89938) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36313 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-1.91032) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36775 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.91495) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49018 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-2.03737) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41302 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-2.96022) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01691 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-2.56410) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38109 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-1.92828) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12875 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-2.67594) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23240 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-1.77960) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49505 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-2.04224) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39181 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-1.93900) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53203 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-2.07922) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.28690 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-2.83409) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73528 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-1.28247) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62047 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-1.16767) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58834 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-1.13553) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47246 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-2.01966) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66477 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-1.21197) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47413 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.02132) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53133 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.07852) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42974 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.97693) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95087 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-2.49806) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28938 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-1.83658) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58074 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-2.12793) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10107 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-2.64827) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32834 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-2.87554) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60046 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-2.14766) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35009 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-1.89729) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46724 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-2.01443) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68444 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-2.23163) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46144 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-2.00864) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75995 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-2.30714) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02356 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.57075) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69726 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-2.24445) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10592 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-1.65312) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37279 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-1.91998) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11900 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-2.66620) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13228 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-2.67948) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04570 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-2.59289) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93533 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-2.48252) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.64946 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-3.19666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03865 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-2.58584) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08608 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-2.63327) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44754 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.99473) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53510 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-2.08230) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36422 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.91141) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98251 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-2.52971) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09636 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-2.64356) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23925 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-2.78645) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07816 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-2.62535) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.89649 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-3.44368) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.52116 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-3.06836) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48261 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-2.02981) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35300 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.90020) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51442 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-2.06162) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29319 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.84039) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14023 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-2.68742) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37445 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-1.92164) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23284 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-1.78003) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14884 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-1.69603) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98159 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-2.52878) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95253 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-2.49972) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02393 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-2.57112) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57214 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-2.11933) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39034 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-1.93753) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20710 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-1.75429) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43973 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-1.98692) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15259 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.69979) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10729 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.65448) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69924 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-2.24644) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64259 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-2.18978) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60289 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-2.15008) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37488 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-1.92208) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19711 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-1.74430) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00723 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.55442) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24527 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.79247) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42294 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.97013) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39178 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.93897) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20223 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.74942) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98023 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-2.52742) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06300 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-2.61020) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13341 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.68060) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94531 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-2.49251) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.53229 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-3.07949) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45782 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-2.00502) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42277 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-1.96997) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39815 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-1.94534) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35213 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-1.89933) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07291 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-2.62010) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23009 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-1.77728) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18734 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-1.73454) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28166 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-1.82885) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98892 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.53611) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73209 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-2.27928) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98159 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-2.52878) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25017 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.79737) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25659 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.80379) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12652 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-2.67371) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15627 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.70346) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29978 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.84697) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29224 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.83944) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94820 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-2.49539) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11062 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-2.65782) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38068 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.92787) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34117 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.88836) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16855 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-0.71574) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15559 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-1.70278) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14870 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-1.69590) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46817 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.01537) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26256 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.80976) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42812 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.97531) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20104 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.74823) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34251 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-0.88970) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39783 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-0.94502) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31230 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-0.85950) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30305 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-0.85025) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10207 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-0.64926) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06132 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-2.60851) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93049 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-1.47769) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88012 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-1.42732) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88004 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-1.42724) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15768 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-1.70487) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99754 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-1.54474) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18922 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-1.73641) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13774 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.68493) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14938 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.69658) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47015 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-2.01734) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62351 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-2.17071) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77179 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-2.31898) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65464 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-2.20184) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26873 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.81592) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13926 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.68645) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22367 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.77086) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31227 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.85946) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27458 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.82178) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53878 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-2.08597) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62199 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-2.16918) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53905 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-2.08624) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81822 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.36541) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77571 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-1.32291) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92881 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-1.47600) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51733 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-2.06453) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85457 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-1.40177) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99871 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.54591) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31266 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.85985) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38607 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.93327) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17967 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-1.72686) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03063 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-1.57783) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20179 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-1.74898) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41761 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.96481) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26107 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.80826) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29413 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.84132) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32316 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-0.87036) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15048 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-0.69767) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27462 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.82181) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59506 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-1.14225) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59620 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-1.14340) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31285 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.86004) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08114 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-1.62833) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86015 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-1.40735) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54234 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-2.08954) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66613 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-2.21332) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58400 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-2.13120) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54210 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-2.08929) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08786 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.63505) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13812 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.68531) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19929 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.74648) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03719 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.58438) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12446 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.67165) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18076 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.72795) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40796 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-2.95516) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04240 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-2.58960) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54183 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-1.08903) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24313 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.79033) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49802 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-1.04522) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23932 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.78652) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26286 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.81006) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26308 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.81027) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15557 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.70276) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91876 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.46596) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00949 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-1.55668) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18266 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.72986) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01945 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-1.56664) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03115 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.57834) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79525 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.34245) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80600 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.35320) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00040 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.54759) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86905 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.41624) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29366 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.84085) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79640 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-1.34359) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18130 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-1.72849) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14225 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-1.68945) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05207 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-1.59927) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89038 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-1.43758) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25287 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.80006) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.43841 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-2.98561) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14612 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-1.69331) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02462 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-1.57181) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90793 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.45513) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89199 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.43918) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90012 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-2.44731) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26563 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.81282) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90418 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.45137) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89585 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-1.44305) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01098 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-1.55818) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30846 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-1.85565) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17882 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.72602) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41539 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-2.96259) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15510 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.70229) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20941 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.75660) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24272 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.78991) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56553 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-2.11272) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42177 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.96896) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13910 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.68629) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18806 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.73525) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33233 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.87953) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67068 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.21787) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18448 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-1.73168) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34607 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.89326) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76420 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.31140) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63430 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.18149) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86470 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.41189) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49488 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-2.04208) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04138 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-1.58857) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05319 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-1.60038) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93634 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.48354) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37812 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-1.92531) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73873 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-2.28592) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42316 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.97036) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29952 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-0.84671) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04269 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-1.58988) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49295 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-2.04015) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49872 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-2.04592) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49065 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.03784) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67528 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.22247) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37235 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-1.91955) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79827 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-1.34547) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96192 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-1.50912) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62634 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-2.17354) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29045 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-1.83764) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29679 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.84399) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15442 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-0.70162) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54760 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.09480) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86203 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.40922) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24738 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.79457) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32392 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-0.87112) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77182 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-1.31902) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18348 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-1.73067) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40820 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.95539) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40428 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.95147) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99294 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.54014) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67982 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-1.22702) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64616 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-1.19336) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44522 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.99242) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95768 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-1.50487) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15379 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.70098) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75464 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-2.30184) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27652 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-0.82372) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19372 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-0.74091) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33394 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.88113) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95798 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-1.50517) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36815 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-2.91535) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42776 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.97496) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25119 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.79838) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28518 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-0.83237) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01640 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-1.56359) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23863 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-1.78583) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19072 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-1.73791) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84208 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.38928) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10786 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-1.65505) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76637 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-2.31357) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48925 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-2.03645) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.29052 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-2.83771) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36842 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-2.91562) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34585 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-1.89304) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47173 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-2.01892) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23405 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-2.78125) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68615 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-2.23335) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43252 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.97971) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53294 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.08014) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67491 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.22210) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28820 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-0.83539) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15083 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-0.69803) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01282 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-0.56001) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38632 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.93351) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08855 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-0.63574) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85514 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-1.40234) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39627 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-1.94346) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12578 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-2.67297) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22369 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (0.22912) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50187 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-0.04906) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09614 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-0.64333) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95695 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.50415) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02444 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-0.57163) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70970 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.25689) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64945 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-2.19664) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30277 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.84997) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19494 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.74214) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07423 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.62143) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10158 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.64877) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75920 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-1.30639) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27972 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-1.82692) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01487 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-2.56206) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67257 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-2.21977) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42141 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-1.96861) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27858 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-1.82578) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01620 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-2.56339) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03652 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-0.58371) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18444 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.73163) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12079 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.66799) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92200 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-1.46920) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09931 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-1.64651) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21268 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-1.75987) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73628 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-2.28347) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11401 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.66120) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77627 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.32346) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21344 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-1.76063) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77729 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.32449) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74714 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.29434) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72241 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.26960) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91586 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.46306) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91042 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.45761) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66693 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.21413) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81861 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.36580) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88544 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.43263) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65874 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.20594) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78689 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-2.33408) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02337 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-1.57056) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72783 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.27503) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31249 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-1.85968) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44501 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.99221) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74467 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-1.29186) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80464 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-1.35183) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96939 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.51658) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93997 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.48717) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99586 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.54306) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06381 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.61100) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88035 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.42755) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13641 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-0.68360) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00152 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-0.54872) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51715 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.06435) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62415 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.17134) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48602 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.03322) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90228 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-0.44948) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03557 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.58276) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01039 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-0.55759) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13238 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.67958) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02863 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.57582) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89488 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.44208) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39644 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.94364) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65715 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.20435) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52646 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.07365) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95586 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.50306) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47634 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.02353) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49487 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-1.04206) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53585 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-1.08304) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46115 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-1.00835) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26904 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-0.81623) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55522 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-1.10241) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41024 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-0.95743) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12048 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-1.66768) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94532 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-1.49252) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20108 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-1.74828) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82190 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.36910) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40013 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.94733) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72725 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-1.27445) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88756 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-0.43476) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87717 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.42436) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70857 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.25576) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81777 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.36496) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44659 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.99379) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56855 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-1.11575) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86268 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.40988) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46521 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.01240) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43487 HOMO: -6.54978 LUMO: 0.29116 factor:1 | -1 (0.01793) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38695 HOMO: -7.18108 LUMO: 0.00000 factor:1 | -1 (0.06585) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79505 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-2.34225) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68200 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.22919) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35855 HOMO: -6.40828 LUMO: 0.02449 factor:1 | -1 (0.09426) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27499 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-1.82218) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51751 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.06470) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39168 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.93887) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98911 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.53630) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80273 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-2.34992) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79709 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-2.34429) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67826 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-2.22546) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89928 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-1.44648) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51597 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-2.06317) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58924 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.13644) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97396 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-0.52115) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32588 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.87308) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58692 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.13412) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02170 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-2.56889) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76858 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-2.31577) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53179 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.07899) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50638 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-1.05357) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69343 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.24062) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95043 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-2.49762) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11035 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-2.65755) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83671 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-2.38391) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94077 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-2.48796) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94918 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-2.49637) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65637 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-1.20356) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68208 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-1.22927) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60724 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-2.15443) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62332 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.17052) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08071 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.62790) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35739 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-0.90459) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03836 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-1.58555) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94184 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.48903) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15096 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-1.69815) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74510 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.29230) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78445 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-1.33164) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99820 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-1.54539) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00549 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-1.55268) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48705 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-2.03424) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47769 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-2.02488) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39281 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.94001) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74270 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-2.28989) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74777 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.29496) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63441 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-1.18160) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01576 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-2.56296) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84836 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.39555) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86575 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.41294) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87905 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.42624) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24289 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.79008) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87612 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-1.42332) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99022 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-1.53742) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73756 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.28476) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57568 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-1.12288) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47002 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-1.01722) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27714 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.82433) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25888 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.80607) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72705 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-2.27425) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92795 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-2.47515) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82840 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-1.37559) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66945 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-1.21665) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85944 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-1.40664) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98442 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-2.53161) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69879 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-1.24598) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62039 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-1.16759) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70792 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-2.25512) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76717 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-1.31436) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72069 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-1.26789) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54665 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-1.09384) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61136 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-1.15855) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79669 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-1.34389) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73795 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-1.28514) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77229 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-1.31948) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42817 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.97536) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99520 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-1.54240) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87495 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-1.42215) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27042 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-1.81761) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51178 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-2.05898) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65054 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-1.19774) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57691 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-1.12410) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58088 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.12808) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.73640 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-3.28360) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81728 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-2.36448) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78720 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.33439) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55862 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-1.10582) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46303 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.01022) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60066 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-2.14785) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50903 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-2.05623) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21602 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-1.76322) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29377 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-1.84096) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76901 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-2.31621) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79900 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-2.34619) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78296 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-3.33016) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64841 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-2.19561) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68338 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-2.23057) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97693 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-2.52413) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88734 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-1.43453) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35450 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-1.90169) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79824 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-2.34543) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85439 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.40159) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86987 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-1.41706) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47465 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-1.02184) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38893 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.93613) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71141 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-1.25861) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29782 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.84501) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74351 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-2.29071) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60503 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.15222) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76742 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.31461) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34177 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-0.88897) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26813 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.81533) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04260 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-2.58979) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68822 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-2.23542) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60485 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-1.15205) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39549 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.94268) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39271 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-1.93990) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.60152 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-3.14871) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03590 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-2.58310) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73949 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-2.28668) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61262 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-3.15981) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43544 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-0.98263) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43416 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-0.98135) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42163 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.96883) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53721 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-1.08440) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34357 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.89076) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78440 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-1.33159) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67321 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-1.22040) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41964 HOMO: -6.38379 LUMO: 0.45443 factor:1 | -1 (0.03317) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34244 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (0.11037) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47749 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.02468) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55596 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.10316) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42698 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.02582) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56195 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.10914) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70699 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-0.25418) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43716 HOMO: -6.70489 LUMO: 0.19048 factor:1 | -1 (0.01565) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62024 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.16743) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33904 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (0.11377) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63880 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.18599) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36739 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.08542) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35664 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (0.09617) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58418 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.13138) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53659 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.08378) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62002 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.16721) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49602 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.04321) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58473 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.13192) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38916 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (0.06365) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42853 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (0.02427) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59458 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.14177) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10642 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.65362) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21894 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.76614) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10090 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.64809) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00433 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.55152) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52228 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.06947) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52810 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.07529) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50668 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.05388) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38070 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.07211) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69578 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.24297) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75922 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-1.30642) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77558 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-1.32277) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43416 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.98135) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69012 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.23731) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45999 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.00718) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76682 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-1.31401) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26639 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-1.81358) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79923 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-1.34642) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57596 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.12316) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39977 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (0.05303) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97101 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-1.51820) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55367 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-1.10086) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19203 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.73922) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47217 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-1.01937) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93327 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.48046) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08479 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.63198) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42156 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.96875) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73141 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.27861) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66227 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.20946) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77251 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.31971) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79357 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.34077) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80255 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.34975) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80772 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.35492) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64862 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.19581) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58701 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.13421) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99351 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-1.54071) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64345 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.19064) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12250 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-1.66969) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66812 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-1.21531) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70837 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-1.25556) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72290 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.27009) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26704 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-1.81424) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84968 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-1.39687) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85664 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.40384) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37368 HOMO: -6.11440 LUMO: 1.89119 factor:1 | -1 (0.07913) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30183 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.84902) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48804 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-1.03523) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58243 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.12963) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63204 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.17923) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70747 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.25466) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68679 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.23398) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37217 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.91936) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90489 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-1.45208) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44545 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.99264) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63572 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.18291) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69776 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.24496) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60943 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.15663) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69825 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.24545) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68810 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-0.23530) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63520 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-0.18240) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46067 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.00786) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03378 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.41903) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81314 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.36033) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23146 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.77865) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72530 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.27249) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66135 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-1.20854) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33690 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-1.88409) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85471 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.40190) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56591 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (0.88690) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72966 HOMO: -6.70216 LUMO: 0.01361 factor:1 | -1 (0.72314) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81116 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (0.64164) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72782 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-1.27502) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20824 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.75543) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70322 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.25042) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88276 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.42996) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82004 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-1.36724) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17386 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.27894) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05703 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (1.39578) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44315 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (1.00965) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44677 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (1.00603) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02102 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (0.43179) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18349 HOMO: -6.90081 LUMO: -0.20136 factor:1 | -1 (0.26931) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23961 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-2.78680) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62603 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.17323) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69318 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-1.24038) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00396 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-2.55115) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66842 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-1.21561) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.75406 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-3.30126) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32900 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-2.87619) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58377 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.13097) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05144 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (0.40137) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23066 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (1.22214) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48786 HOMO: -6.39468 LUMO: -1.06941 factor:1 | -1 (0.96494) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16174 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-1.70893) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72733 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-1.27453) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52611 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.07331) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95477 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.50197) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51066 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.05785) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46888 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-1.01607) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78075 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-1.32794) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53623 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-1.08342) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91179 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-2.45898) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69172 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-3.23892) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06292 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-2.61012) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66840 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.21560) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66339 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.21059) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64086 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.18806) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53645 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.08365) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14437 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-2.69156) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37604 HOMO: -4.69941 LUMO: 1.14016 factor:1 | -1 (0.07676) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51188 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.05908) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04089 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-1.58808) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64753 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.19472) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73158 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.27877) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44324 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.99043) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67490 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.22209) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14384 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.69103) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42262 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.96981) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48701 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.03420) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55126 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.09845) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37165 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-0.91885) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72203 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-1.26922) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18087 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.72806) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36850 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.91569) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68314 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.23034) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30628 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.85348) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13920 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.68640) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67785 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-2.22505) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39105 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.93825) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39756 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.94475) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41616 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.96336) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53341 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-0.08060) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84876 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.39595) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10626 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.65345) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99371 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.54091) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34624 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.89343) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46088 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.00807) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37183 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-1.91903) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71853 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-2.26573) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23582 HOMO: -5.37153 LUMO: 1.05580 factor:1 | -1 (0.21698) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66508 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-0.21228) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00414 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.55133) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28373 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.83093) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66950 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-2.21669) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30911 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.85631) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22466 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.77185) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05497 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.60216) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32577 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.87297) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57121 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-2.11841) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68207 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-2.22927) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40120 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.94839) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56727 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-2.11446) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33960 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.88679) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51680 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-1.06399) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59088 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.13807) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63028 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.17747) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52802 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.07521) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45730 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-0.00449) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48143 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.02863) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30576 HOMO: -4.87084 LUMO: 1.41771 factor:1 | -1 (0.14705) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75873 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.30593) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53453 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-2.08173) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44818 HOMO: -4.81369 LUMO: 1.14288 factor:1 | -1 (0.00463) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33867 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-0.88587) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53800 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.08519) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26741 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-0.81460) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48851 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-0.03570) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48024 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-0.02743) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21422 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (0.23859) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48881 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-0.03600) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39384 HOMO: -5.43411 LUMO: 0.45987 factor:1 | -1 (0.05897) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09060 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (0.36221) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42127 HOMO: -5.33071 LUMO: 1.14016 factor:1 | -1 (0.03154) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26622 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (0.18659) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34763 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.89482) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33508 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.88227) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01112 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.55831) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86472 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.41192) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42028 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.96747) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06156 HOMO: -7.68722 LUMO: 0.71838 factor:1 | -1 (0.39125) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39917 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (0.05363) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12909 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.67628) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06043 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.60762) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41734 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-0.96453) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74290 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.29009) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43456 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.98175) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34357 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-0.89076) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16779 HOMO: -6.91713 LUMO: 0.33198 factor:1 | -1 (0.28501) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34619 HOMO: -6.83278 LUMO: 0.26667 factor:1 | -1 (0.10661) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11568 HOMO: -6.89264 LUMO: -1.00682 factor:1 | -1 (0.33712) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20760 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.75479) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92527 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.47246) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40559 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-0.95278) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09655 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.64374) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25375 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-0.80094) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50757 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-1.05477) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86880 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.41600) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15584 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.70303) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09780 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-0.64499) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34232 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-0.88951) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83490 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-1.38209) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61764 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-2.16483) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88540 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.43260) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76642 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-3.31361) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69510 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-0.24229) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40930 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.95650) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74324 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-2.29044) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87983 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-1.42702) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48623 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-2.03343) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94897 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.49616) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66152 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-0.20871) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18390 HOMO: -7.15932 LUMO: -2.52794 factor:1 | -1 (0.26890) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70059 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.24779) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35724 HOMO: -6.57427 LUMO: -2.78645 factor:1 | -1 (0.09557) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78537 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-1.33257) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00108 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.54827) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12885 HOMO: -7.47769 LUMO: -0.43810 factor:1 | -1 (0.32395) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72841 HOMO: -6.68040 LUMO: -2.22589 factor:1 | -1 (0.72439) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49263 HOMO: -6.92802 LUMO: -1.99187 factor:1 | -1 (0.96018) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03386 HOMO: -7.73620 LUMO: 0.01633 factor:1 | -1 (0.41895) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63445 HOMO: -7.28721 LUMO: -0.18504 factor:1 | -1 (0.81836) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53792 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.08512) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50791 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-0.05510) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.55222 HOMO: -7.36612 LUMO: 0.16055 factor:1 | -1 (0.90059) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56403 HOMO: -7.67633 LUMO: 0.33198 factor:1 | -1 (0.88878) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68534 HOMO: -7.07768 LUMO: -0.27483 factor:1 | -1 (0.76747) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15723 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-0.70442) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07940 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.62660) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73420 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.28139) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81057 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.35777) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90644 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.45363) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35926 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.90646) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94154 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.48873) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12603 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-2.67322) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57826 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-2.12545) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94638 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.49358) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25145 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.79865) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02327 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.57046) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25859 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.80578) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44026 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (0.01254) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86315 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.41035) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.26265 HOMO: -7.59470 LUMO: -1.21363 factor:1 | -1 (3.19015) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.25883 HOMO: -7.23279 LUMO: -1.23812 factor:1 | -1 (2.19397) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.98307 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (2.46973) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.92422 HOMO: -7.36340 LUMO: -0.17143 factor:1 | -1 (2.52859) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95915 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.50634) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60925 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-2.15645) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32476 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.87195) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05647 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (0.39633) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65616 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.20335) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36559 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (0.08721) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24704 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (1.20576) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78458 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (0.66823) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.40397 HOMO: -7.22462 LUMO: 0.04354 factor:1 | -1 (1.04884) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34709 HOMO: -7.16204 LUMO: -0.23674 factor:1 | -1 (0.10572) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76206 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-0.30926) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48673 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.03392) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34750 HOMO: -6.63141 LUMO: -0.22858 factor:1 | -1 (0.10531) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39449 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (0.05831) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41844 HOMO: -6.60148 LUMO: -1.13744 factor:1 | -1 (0.03437) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30928 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.85648) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43005 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-0.97724) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11440 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.66159) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27598 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-0.82317) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06575 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-2.61295) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63685 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-2.18404) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60349 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-2.15068) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46823 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-0.01543) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19362 HOMO: -7.06680 LUMO: -0.89253 factor:1 | -1 (0.25919) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55360 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.10079) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83115 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.37835) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63237 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.17957) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70527 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.25247) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73610 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-0.28330) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18525 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.73245) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72595 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.27315) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75727 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-1.30446) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18252 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-2.72971) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31758 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.86477) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59870 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-2.14589) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21562 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.76282) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27815 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.82535) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56804 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-1.11523) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70388 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-1.25107) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12454 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-1.67173) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72472 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.27191) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51372 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.06092) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71667 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.26386) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77533 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.32253) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54997 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.09716) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52684 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.07403) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75569 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.30288) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66012 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-1.20731) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83865 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.38585) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56436 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-2.11155) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95409 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.50128) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36788 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-2.91507) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87427 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-2.42146) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37991 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-2.92710) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79101 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.33820) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87247 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-2.41966) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06089 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.60808) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72490 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-2.27210) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51083 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-2.05802) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35523 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-2.90242) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68577 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-2.23297) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.72002 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-3.26722) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61433 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-3.16153) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02360 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-2.57080) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82217 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.36937) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64455 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.19174) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66468 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-2.21188) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71956 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-0.26675) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58531 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-2.13250) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58542 HOMO: -7.33891 LUMO: -0.96873 factor:1 | -1 (0.86739) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32560 HOMO: -7.36068 LUMO: -0.28028 factor:1 | -1 (1.12720) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63527 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-2.18246) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10198 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.64917) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88962 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-1.43682) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59191 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.13910) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35623 HOMO: -6.52801 LUMO: -1.17553 factor:1 | -1 (0.09657) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22428 HOMO: -7.54844 LUMO: -1.18642 factor:1 | -1 (0.22852) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66912 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-2.21631) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80418 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-1.35137) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11787 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-1.66506) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11240 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-1.65960) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65615 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-1.20334) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62076 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-2.16796) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21868 HOMO: -6.06270 LUMO: 0.16327 factor:1 | -1 (0.23413) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55345 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-1.10065) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50725 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.05444) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71365 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-1.26084) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79455 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-1.34174) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99844 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.54563) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01414 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.56133) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80663 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-1.35382) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23377 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.78097) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28267 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.82987) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35486 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.90206) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62310 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-2.17030) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78282 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-1.33001) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87999 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-1.42718) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86683 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.41402) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08460 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.63179) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36660 HOMO: -6.60148 LUMO: -0.61770 factor:1 | -1 (0.08621) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41340 HOMO: -6.55794 LUMO: -1.06941 factor:1 | -1 (0.03940) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17468 HOMO: -7.12666 LUMO: -0.11973 factor:1 | -1 (0.27813) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24635 HOMO: -7.21646 LUMO: -0.50069 factor:1 | -1 (0.20645) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60270 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-2.14989) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94111 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-1.48830) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89147 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-1.43867) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52232 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.06952) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49865 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-1.04584) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66622 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-1.21341) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92445 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.47165) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92530 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.47249) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24215 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.78934) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93800 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-1.48520) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86777 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-1.41496) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47788 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-2.02507) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48114 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-2.02834) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65540 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-2.20260) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74551 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.29270) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05529 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.60249) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04297 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.59016) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12708 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.67427) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93691 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-2.48410) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04411 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.59130) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65752 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-3.20471) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17819 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-2.72538) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65887 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.20606) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56180 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-2.10899) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85871 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.40590) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99242 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-2.53961) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37841 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-2.92560) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.48971 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-3.03690) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90556 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-2.45275) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14026 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-2.68745) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27081 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-0.81800) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43021 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.97741) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17140 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.71860) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81957 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-2.36676) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90477 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-2.45196) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74628 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.29347) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82911 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.37631) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76410 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.31130) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59256 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.13976) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82670 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-2.37389) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01362 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-2.56081) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92937 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-2.47656) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27710 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-2.82430) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24264 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.78984) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19336 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-0.74056) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16683 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.71403) | -1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23779 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (1.21502) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51676 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (0.93604) | 1 | -1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66343 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (0.78938) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96169 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (0.49111) | 1 | 1 |
| G: -5246.08711 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15993 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (0.29288) | 1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33351 HOMO: -6.74570 LUMO: -2.85447 factor:1 | -1 (0.11929) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51155 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-1.05874) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77697 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-1.32416) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89188 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-1.43907) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06677 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-1.61396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18851 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-1.73571) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40740 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-1.95459) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22338 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.77057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36741 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-0.91460) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22022 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.76742) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72807 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.27526) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73932 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-2.28652) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79947 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.34666) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35202 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-1.89922) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40683 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-1.95402) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54348 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-2.09068) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53068 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-1.07787) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82287 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.37007) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86630 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-1.41350) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63633 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-2.18352) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07240 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.61959) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42621 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.97341) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57666 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-1.12386) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39364 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.94083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62302 HOMO: -7.08857 LUMO: -0.89798 factor:1 | -1 (0.82978) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56920 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (0.88361) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27879 HOMO: -6.59332 LUMO: -0.60137 factor:1 | -1 (0.17402) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18559 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (0.26722) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49248 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.03967) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26244 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.19037) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11315 HOMO: -6.86271 LUMO: -1.03947 factor:1 | -1 (0.33965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52266 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.06985) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56953 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.11673) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56265 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-1.10984) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39355 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (1.05926) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29183 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (1.16097) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07402 HOMO: -6.74298 LUMO: -0.85172 factor:1 | -1 (0.37878) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96531 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (0.48749) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65293 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.20012) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85368 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-1.40087) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78641 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-1.33360) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23230 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.77950) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55168 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-1.09888) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43908 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.98628) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30508 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.14773) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21803 HOMO: -6.94707 LUMO: -2.62318 factor:1 | -1 (0.23478) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29305 HOMO: -7.28177 LUMO: -0.09796 factor:1 | -1 (0.15976) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15185 HOMO: -6.80013 LUMO: -0.79729 factor:1 | -1 (0.30096) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50131 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-2.04850) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63351 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-1.18070) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80323 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-1.35042) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73705 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-1.28424) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53381 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-1.08100) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57318 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-1.12037) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54181 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-1.08900) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38588 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.93308) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75773 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-1.30492) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67310 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-1.22029) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50036 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-1.04756) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57419 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-1.12138) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60597 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-1.15316) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43209 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.97928) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36553 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.91272) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48602 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-1.03322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45472 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-2.00191) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54134 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-1.08854) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52893 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.07613) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66056 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.20775) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25139 HOMO: -6.26134 LUMO: 1.53744 factor:1 | -1 (0.20142) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20377 HOMO: -5.97562 LUMO: 1.42316 factor:1 | -1 (0.24904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38761 HOMO: -6.65046 LUMO: 1.44492 factor:1 | -1 (0.06520) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48755 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.03475) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73294 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.28013) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71449 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-1.26168) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03101 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-1.57821) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08435 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.63154) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25923 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.80643) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37594 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.92314) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39761 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.94481) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31405 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.86124) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48254 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-1.02973) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61862 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.16582) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27114 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (0.18166) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25184 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.79904) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70244 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.24964) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99159 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.53879) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78959 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.33679) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33900 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.88619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65870 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-2.20589) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36593 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.91312) | 1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86968 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.41687) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21165 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.75884) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20479 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.75199) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44014 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.98734) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09642 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-2.64361) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61483 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-2.16203) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68425 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-2.23144) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49831 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-2.04551) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13558 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-2.68277) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70019 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-2.24739) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55884 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-1.10603) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11054 HOMO: -6.80013 LUMO: -2.54154 factor:1 | -1 (0.34226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47313 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.02033) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40677 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-2.95396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38283 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-1.93002) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50847 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.05567) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38169 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-0.92889) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44735 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.99455) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69147 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.23866) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66847 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.21567) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49556 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-2.04276) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69242 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-1.23961) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80216 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.34936) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36680 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.91399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26065 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-1.80784) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89855 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.44574) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19134 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.73854) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33668 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.88387) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49367 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.04086) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57947 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.12666) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51614 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-2.06333) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82129 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-2.36848) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19773 HOMO: -6.77564 LUMO: 0.23402 factor:1 | -1 (0.25508) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22110 HOMO: -7.07224 LUMO: -0.75648 factor:1 | -1 (0.23170) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44252 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-2.98971) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44307 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.99027) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53916 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-2.08635) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78934 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-2.33653) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22077 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.76796) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99897 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.54616) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10112 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-0.64831) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27775 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.82494) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20120 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-0.74839) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22468 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.77188) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09601 HOMO: -6.91169 LUMO: -1.48574 factor:1 | -1 (0.35680) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46614 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.01333) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23841 HOMO: -6.78652 LUMO: -1.51840 factor:1 | -1 (0.21440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21524 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.76244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99143 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.53862) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25873 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.80592) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09736 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.64456) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21347 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.76067) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36273 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.90992) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08790 HOMO: -7.08040 LUMO: -1.09662 factor:1 | -1 (0.36490) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34162 HOMO: -6.90897 LUMO: -1.14016 factor:1 | -1 (0.11119) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26320 HOMO: -6.68312 LUMO: -0.74831 factor:1 | -1 (0.18961) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38510 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.93229) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34825 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.89545) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46986 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.01705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03472 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.58192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86977 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-0.41696) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89050 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-0.43770) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99771 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.54491) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06974 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.61694) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05908 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.60627) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11407 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.66126) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81656 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.36375) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11523 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.66243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61011 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.15730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79689 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.34408) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90998 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.45717) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65532 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-2.20252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51548 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-2.06268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41363 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.96083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65945 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-3.20664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69883 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-2.24603) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06692 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-2.61412) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45690 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-2.00409) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59804 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-2.14524) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51059 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-2.05778) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72647 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.27366) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79771 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.34490) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79142 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.33862) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88692 HOMO: -6.90353 LUMO: -0.90070 factor:1 | -1 (0.56589) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11843 HOMO: -7.39061 LUMO: 0.17687 factor:1 | -1 (0.33437) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06428 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (0.38852) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93690 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.48409) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08131 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.62850) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89558 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-1.44277) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12350 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-1.67070) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41061 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.95780) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40419 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.95138) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74624 HOMO: -6.94435 LUMO: 1.74969 factor:1 | -1 (0.70657) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02080 HOMO: -7.02598 LUMO: 1.43404 factor:1 | -1 (0.43201) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88320 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.43039) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85539 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.40258) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03289 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.58008) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08364 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-1.63083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39015 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.93734) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06602 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-2.61322) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55001 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-2.09721) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64447 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-2.19166) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81199 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.35918) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94636 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.49355) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97950 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-1.52669) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99219 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-0.53938) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13853 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.68573) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33024 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.87743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44700 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.99420) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10774 HOMO: -7.23823 LUMO: -0.06259 factor:1 | -1 (0.34507) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33732 HOMO: -6.76475 LUMO: -0.99049 factor:1 | -1 (0.11549) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96726 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.51446) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94882 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.49601) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98155 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.52874) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01524 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.56243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82245 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.36964) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89230 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.43949) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60171 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.14890) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89897 HOMO: -7.07768 LUMO: -0.26939 factor:1 | -1 (0.55383) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59143 HOMO: -7.15932 LUMO: 0.42450 factor:1 | -1 (0.86138) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20867 HOMO: -7.46136 LUMO: 0.04626 factor:1 | -1 (0.24414) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92656 HOMO: -7.05047 LUMO: -1.06669 factor:1 | -1 (0.52624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62561 HOMO: -6.66951 LUMO: -0.99322 factor:1 | -1 (0.82720) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.85222 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.60058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51533 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.06252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63458 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.18177) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88223 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-0.42942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18910 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-2.73630) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10020 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-2.64740) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68923 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-2.23642) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66180 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-2.20899) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39103 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.93822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43228 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-0.97947) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02626 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.57345) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00141 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.54861) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11532 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.66252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90971 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-0.45691) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68744 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-1.23464) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95555 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.50275) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05675 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-1.60395) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07699 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-2.62418) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32430 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.87149) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57891 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-2.12611) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79187 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-2.33906) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40950 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.95670) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96724 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.51443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87616 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.42335) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78612 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.33331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68726 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-0.23445) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00065 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.54785) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94873 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.49593) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73624 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.28343) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81536 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.36256) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72366 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.27085) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97316 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.52035) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00541 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-1.55260) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63696 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.18416) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81553 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-0.36273) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02846 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.57566) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19115 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.73834) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27866 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.82586) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08772 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.63491) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51769 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-2.06488) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52664 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-2.07383) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08685 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.63404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26756 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.81475) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03384 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.58104) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33774 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.88493) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02764 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-1.57483) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09022 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.63742) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57652 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.12371) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34761 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-2.89480) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81682 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.36402) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77650 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-2.32369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93647 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-2.48366) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71724 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.26443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39519 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-0.94238) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55508 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.10228) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52825 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-1.07545) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43509 HOMO: -6.88720 LUMO: 1.68711 factor:1 | -1 (0.01771) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68171 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-0.22890) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63352 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.18071) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77284 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.32003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53158 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.07878) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20319 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.75038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49995 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.04715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46999 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.01719) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68594 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.23314) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40262 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-0.94981) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59893 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-0.14613) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66040 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-0.20760) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56843 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.11562) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64595 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.19315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67365 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-0.22085) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76038 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-0.30757) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62065 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.16784) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60605 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.15325) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89694 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.44414) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97691 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-2.52410) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32448 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-2.87167) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68591 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-2.23310) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94837 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.49556) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31185 HOMO: -6.74298 LUMO: -0.70477 factor:1 | -1 (0.14095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27615 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (0.17666) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60576 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.15296) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47341 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.02060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27838 HOMO: -7.14843 LUMO: -1.19730 factor:1 | -1 (0.17442) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02157 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.56876) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29538 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.84257) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28294 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.83014) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63786 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-1.18506) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46251 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.00971) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34313 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.89032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31382 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.86101) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25589 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-1.80308) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60316 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-2.15035) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55967 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-2.10687) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89033 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.43752) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00013 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.54732) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80227 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-1.34947) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49439 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-2.04159) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28859 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-1.83579) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01759 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-2.56478) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72055 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-2.26774) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58218 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-2.12937) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90312 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-1.45031) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04592 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-1.59312) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84943 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.39662) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70298 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.25017) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73171 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.27891) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45233 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.99953) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57310 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-1.12029) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46863 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-1.01583) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72129 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-1.26849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47817 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.02536) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34701 HOMO: -6.99333 LUMO: 1.87214 factor:1 | -1 (0.10580) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34723 HOMO: -6.65591 LUMO: 1.37962 factor:1 | -1 (0.10558) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08345 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.63064) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11575 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.66294) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45937 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-2.00657) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20116 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.74836) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47819 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.02538) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03820 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.58539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32379 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.87098) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33995 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.88715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03497 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.58216) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59721 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.14440) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71416 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-1.26136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50066 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-1.04786) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15189 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.69909) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70584 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.25304) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66157 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.20877) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65409 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.20128) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69782 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.24501) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84335 HOMO: -6.41644 LUMO: 1.78235 factor:1 | -1 (0.60945) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69915 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.24634) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10986 HOMO: -6.35658 LUMO: 1.59731 factor:1 | -1 (0.34295) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77333 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.32052) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74359 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.29078) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89964 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.44684) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71553 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.26273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32369 HOMO: -6.74842 LUMO: 1.96194 factor:1 | -1 (0.12912) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27014 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (0.18267) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32570 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.12710) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43994 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (0.01287) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49509 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.04229) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37694 HOMO: -5.95929 LUMO: 1.62724 factor:1 | -1 (0.07587) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32510 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (0.12770) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16615 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.71335) | 1 | 1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50580 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-1.05300) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32145 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.86864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18594 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.73313) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34730 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.89449) | 1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41237 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.04044) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61695 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-0.16414) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44358 HOMO: -6.93346 LUMO: 2.22861 factor:1 | -1 (0.00922) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61548 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.16267) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36037 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (0.09244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35100 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.89819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10468 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.65188) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49555 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-1.04274) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49089 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-1.03809) | 1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39533 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.94252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12732 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.67452) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47165 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.01885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27429 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.82148) | 1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07339 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.62058) | 1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36852 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-0.91572) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78236 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.32956) | 1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71869 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-0.26588) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91154 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.45873) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76174 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.30893) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23992 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.78712) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40330 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.95049) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47900 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-1.02620) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29266 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.83985) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24928 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.79648) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32257 HOMO: -6.63686 LUMO: -0.52790 factor:1 | -1 (0.13023) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27378 HOMO: -6.75114 LUMO: -0.13334 factor:1 | -1 (0.17902) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52459 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.07178) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42298 HOMO: -6.74298 LUMO: -0.84627 factor:1 | -1 (0.02982) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29400 HOMO: -7.15932 LUMO: 0.22041 factor:1 | -1 (0.15881) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39014 HOMO: -6.90081 LUMO: -1.16737 factor:1 | -1 (0.06267) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41642 HOMO: -7.04775 LUMO: -0.84355 factor:1 | -1 (0.03638) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55955 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-1.10674) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54246 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.08965) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48942 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-1.03662) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69367 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.24087) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50317 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-1.05036) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39182 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.93901) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46763 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-1.01482) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41130 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.95849) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21505 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.76225) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21902 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-0.76622) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07165 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-0.61884) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20947 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-0.75667) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05489 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-0.60208) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02169 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.56888) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04563 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.59283) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83046 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.37766) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83607 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.38326) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33660 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.88380) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46795 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.01515) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28655 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.83375) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06953 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-2.61673) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98809 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-2.53528) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81963 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-2.36682) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49790 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-2.04510) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46027 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.00747) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07343 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.62063) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95983 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-1.50702) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24342 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-1.79062) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55329 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.10048) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37837 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-0.92557) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08906 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.63626) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86900 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.41620) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59079 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.13798) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21249 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.75969) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88715 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-0.43435) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92337 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.47057) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46194 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.00913) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47451 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.02171) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21668 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-0.76388) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32205 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-0.86924) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27513 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.82233) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89034 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.43753) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13263 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.67982) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41111 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.95830) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47481 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-1.02201) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22621 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.77340) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26139 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.80859) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08748 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.63468) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42335 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.97055) | 1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57245 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.11964) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20311 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.75030) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55604 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-1.10323) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27528 HOMO: -6.70489 LUMO: -0.83539 factor:1 | -1 (0.17753) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67278 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-0.21998) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43305 HOMO: -6.94162 LUMO: -1.22451 factor:1 | -1 (0.01976) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69197 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.23916) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36720 HOMO: -6.88176 LUMO: 0.11157 factor:1 | -1 (0.08561) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43180 HOMO: -6.91713 LUMO: 1.27621 factor:1 | -1 (0.02101) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18926 HOMO: -6.77836 LUMO: 1.01226 factor:1 | -1 (0.26354) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47191 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.01910) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35863 HOMO: -6.96884 LUMO: 1.48574 factor:1 | -1 (0.09418) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12298 HOMO: -7.24367 LUMO: 1.28438 factor:1 | -1 (0.32983) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08013 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-1.62732) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21070 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.75789) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47655 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.02375) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36542 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.91262) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65546 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-2.20265) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08352 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-2.63072) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07038 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-2.61757) | 1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27681 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.82401) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52027 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-2.06747) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14768 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.69487) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47946 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.02666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26077 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.80796) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40578 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.95297) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04882 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.59601) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88057 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.42776) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08250 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.62970) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55095 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.09814) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29277 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.83996) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44994 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.99713) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20809 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.75528) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00248 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-0.54967) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07368 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.62087) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99009 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.53728) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45989 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-2.00708) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28217 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-1.82937) | -1 | -1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.91983) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01745 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-2.56465) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30857 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-1.85576) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41864 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-1.96583) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75848 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-2.30568) | 1 | 1 |
| G: -5246.08711 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71508 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-2.26227) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32754 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.87474) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42725 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.97444) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41688 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.96407) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89554 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.44273) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01105 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.55824) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93458 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.48178) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07663 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.62382) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02522 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.57242) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21525 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.23756) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92131 HOMO: -7.21918 LUMO: 0.08436 factor:1 | -1 (0.53149) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11451 HOMO: -7.38789 LUMO: 1.02587 factor:1 | -1 (0.33829) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02406 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (0.42874) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74411 HOMO: -7.04231 LUMO: 0.54151 factor:1 | -1 (0.70869) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01475 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.56194) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71444 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.26164) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13396 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.68116) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58614 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.13334) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62579 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.17298) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52932 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.07652) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64407 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.19127) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42698 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.02582) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39531 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (0.05750) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55830 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.10550) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42500 HOMO: -7.26816 LUMO: 0.32926 factor:1 | -1 (0.02781) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50334 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.05053) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13050 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.67769) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99719 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.54438) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24974 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.79693) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10135 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.64855) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32523 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.87242) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16825 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.71544) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20885 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.75604) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12319 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.67038) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37271 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.91991) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87475 HOMO: -6.52801 LUMO: -0.28028 factor:1 | -1 (0.57805) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59622 HOMO: -7.22462 LUMO: 0.52518 factor:1 | -1 (0.85659) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48609 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.96671) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11441 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.33840) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00055 HOMO: -6.71033 LUMO: 1.59187 factor:1 | -1 (0.45225) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00531 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.44749) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.78009 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (1.67271) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.87865 HOMO: -6.55250 LUMO: 1.73064 factor:1 | -1 (1.57415) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.89846 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (1.55434) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.56134 HOMO: -6.84911 LUMO: 1.98099 factor:1 | -1 (1.89146) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.97966 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (1.47314) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45344 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.99937) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.06753 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (1.38528) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86360 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.58921) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21767 HOMO: -6.93618 LUMO: 2.00004 factor:1 | -1 (0.23513) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14015 HOMO: -6.50896 LUMO: 1.73609 factor:1 | -1 (0.31266) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13106 HOMO: -6.69672 LUMO: 2.37283 factor:1 | -1 (0.32175) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21624 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.76343) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81027 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.35747) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12840 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.67560) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96051 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.50770) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02781 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.57500) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32148 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.86867) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04397 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.59117) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27769 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.82489) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06797 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.61517) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03442 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.58162) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06618 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.61337) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07176 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.61895) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05309 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.60028) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14351 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.69071) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07227 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.61947) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95222 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.49941) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92985 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.47704) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11584 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.66303) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06068 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.60788) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58625 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.13344) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59909 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.14629) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04577 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.59296) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06117 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.60836) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08572 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.63291) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89962 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.44681) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93872 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.48591) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58796 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.13516) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86503 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.41223) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67882 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.22602) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02482 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.57201) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15442 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.70162) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87076 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.41796) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67620 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.22340) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66736 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.21455) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60733 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.15452) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70804 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.25523) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72461 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.27181) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86185 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.40904) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53414 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.08133) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42021 HOMO: -6.60692 LUMO: -0.22313 factor:1 | -1 (0.03260) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87807 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.42526) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77017 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.31737) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90394 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.45114) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88114 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.42833) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84879 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.39598) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84027 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.38746) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75131 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.29851) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77975 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.32694) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25551 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.80270) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34247 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.88967) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21393 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.76112) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08478 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.63198) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41122 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.95841) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42629 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.97349) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29639 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.84358) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46472 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.01191) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23746 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.78466) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28922 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.83641) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18448 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.73168) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21412 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.76131) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17126 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.71845) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07080 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.61799) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54954 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.09674) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41966 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.03314) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35444 HOMO: -6.78652 LUMO: 2.05718 factor:1 | -1 (0.09837) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42293 HOMO: -6.87360 LUMO: 2.34290 factor:1 | -1 (0.02988) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91721 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.46441) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05488 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.60207) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18353 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.73073) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03700 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.58419) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95311 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.50030) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75514 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.30234) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09980 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.64700) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20827 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.75546) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86826 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.41545) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11101 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.65821) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03860 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.58580) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92628 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.47347) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99689 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.54408) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89532 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.44251) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04199 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.58918) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11222 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.65941) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05557 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.60276) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08255 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.62974) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28772 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.83492) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25009 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.79728) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93836 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.48555) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01689 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.56408) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97795 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.52514) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90818 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.45537) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86393 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.41113) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06211 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.60931) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68750 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.23469) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54812 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.09531) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76763 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.31483) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65258 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.19978) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61100 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.15820) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72050 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.26770) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72546 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.27265) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72102 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.26821) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47949 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.02669) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40651 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.95370) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16417 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.71136) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23674 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.78393) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22515 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.77234) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06939 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.61658) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25734 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.80453) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30583 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.85302) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27946 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.82665) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21546 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.76265) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13051 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.67770) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19459 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.74178) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23902 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.78622) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03856 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.58575) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23829 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.78548) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96751 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.51470) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37149 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.91868) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08348 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.63068) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26651 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.81370) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10890 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.65609) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10648 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.65367) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02732 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.57451) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00027 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.54747) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97227 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.51947) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02310 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.57030) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10278 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.64997) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08280 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.63000) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98470 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.53189) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23763 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.78482) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09346 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.64066) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06812 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-2.61531) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.88128 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-3.42847) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16932 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.71651) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88412 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-2.43131) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14396 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.69115) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45533 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.00252) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80573 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.35292) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59321 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.14040) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92423 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.47143) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99185 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.53905) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78415 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.33134) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54798 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.09518) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60754 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-2.15473) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46528 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-2.01247) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30057 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.84776) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54814 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-2.09533) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56512 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-2.11231) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34827 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.89546) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80450 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-2.35169) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71100 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-2.25819) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00167 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.54886) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02361 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.57080) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14394 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.69113) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30343 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.85062) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17961 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.72681) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03245 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.57964) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.80993 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-3.35712) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20056 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-2.74775) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01503 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.56222) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24758 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-2.79477) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99615 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.54335) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90771 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-2.45490) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04780 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.59500) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02595 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.57314) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88377 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.43097) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81257 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.35976) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65088 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.19807) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81200 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.35919) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87096 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.41816) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60050 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.14769) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41190 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.95909) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00015 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.54735) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90698 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.45418) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00443 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.55162) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63356 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.18076) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56281 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.11001) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75522 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.30242) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62065 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (0.83215) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71734 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.73547) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50693 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.05412) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07136 HOMO: -6.62597 LUMO: 2.00276 factor:1 | -1 (0.38145) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.37024 HOMO: -7.01237 LUMO: 1.95922 factor:1 | -1 (2.08257) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.77882 HOMO: -7.03959 LUMO: 2.16875 factor:1 | -1 (1.67399) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.62529 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (1.82752) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.34395 HOMO: -6.40012 LUMO: 1.95650 factor:1 | -1 (2.10886) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29455 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (1.15825) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05422 HOMO: -6.95795 LUMO: 2.28848 factor:1 | -1 (1.39858) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.00241 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (1.45039) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.70532 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (1.74749) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46279 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.00999) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41354 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (0.03927) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57569 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.12289) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56152 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.10871) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35084 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.10196) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50287 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.05007) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53373 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.08093) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59126 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.13845) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30749 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.85468) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55577 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.10296) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65557 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-2.20276) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52288 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-2.07008) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18173 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-2.72892) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37777 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.92496) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62773 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-2.17492) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50080 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.04799) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53707 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.08426) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47582 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.02301) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54491 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.09210) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63055 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.17774) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54288 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.09007) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43392 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.01888) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65058 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.19777) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52527 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.07246) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44529 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.99248) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23271 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.77991) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26319 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.81038) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47489 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.02209) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28518 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.83237) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73333 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.28052) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84217 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.38937) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90841 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.45560) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94503 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.49223) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27865 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.17415) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10186 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.35095) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22883 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.22398) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38538 HOMO: -6.67767 LUMO: -0.48436 factor:1 | -1 (0.06743) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34644 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.10637) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33367 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.11913) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31988 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.13293) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52420 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.07139) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59343 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-1.14062) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28776 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.83495) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42953 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.97673) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12398 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.32882) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00602 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.44678) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24799 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.20482) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13002 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.32278) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48557 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.03276) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29210 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.16071) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16412 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.28869) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08589 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.36692) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17797 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.27483) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27071 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.18210) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06322 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (0.38959) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95145 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.49864) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13080 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.67800) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23764 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.78483) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31562 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.86282) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60349 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.15069) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78429 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.33148) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68945 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-2.23664) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44396 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.99116) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32606 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.87325) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59230 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.13950) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68131 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.22850) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35938 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.90657) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40031 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.94750) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22550 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.77269) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48994 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.03713) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21127 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.75846) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34150 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.88870) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53259 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.07978) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62456 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.17176) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53776 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.08495) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74598 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.29318) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66024 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.20743) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56309 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.11029) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39633 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.94353) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40123 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.94843) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56398 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.11118) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52733 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.07452) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76116 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.30835) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21340 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-2.76060) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43945 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.98665) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59434 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.14154) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54155 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-2.08875) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68564 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-2.23283) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61381 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.16100) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80170 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.34890) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92908 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.47627) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70889 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.25609) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54162 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.08882) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89306 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.44025) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99039 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.53759) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20689 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.75408) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17862 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.72581) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05788 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.60507) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25312 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.80031) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29647 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.84366) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84546 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.39265) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54828 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.09548) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20459 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.75179) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82763 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-1.37483) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54534 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.09254) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50643 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-1.05362) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61767 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.16487) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87934 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.42653) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58328 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.13047) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64189 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-1.18908) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38412 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.93131) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48175 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-1.02894) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74905 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-1.29624) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65694 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-1.20413) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16251 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.70970) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12125 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.66845) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09021 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.63740) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14169 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.68888) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17432 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.72151) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96291 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.51010) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23500 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.78219) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99975 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-1.54694) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09700 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-1.64419) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84519 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-1.39238) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03694 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-1.58414) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03787 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-1.58506) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46436 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-1.01156) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67914 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-1.22634) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61756 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-1.16476) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57272 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-1.11991) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65737 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-1.20457) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63457 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-1.18176) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57283 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-1.12002) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79591 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-1.34310) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08486 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.63206) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70028 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-1.24748) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89411 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-1.44131) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82875 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-1.37594) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93746 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-1.48465) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91210 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.45929) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59053 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.86227) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74901 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.70380) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73614 HOMO: -6.58243 LUMO: 2.20684 factor:1 | -1 (0.71667) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03737 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.41544) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90480 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (0.54801) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.82983 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (0.62298) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96698 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-1.51418) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28538 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-1.83258) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17969 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-1.72689) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01771 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.56491) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89154 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.43873) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12983 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.67702) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25345 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-0.80064) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13132 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.67852) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10240 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.64959) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02400 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.57119) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03390 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-1.58109) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15771 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-1.70490) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13774 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-1.68493) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22013 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-1.76733) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54939 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-2.09658) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39447 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.94167) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33744 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.88463) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.57134 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-3.11853) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56642 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-2.11362) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54052 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-2.08771) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57742 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-2.12461) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61663 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-2.16382) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56936 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-2.11656) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48024 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.02744) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39115 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-1.93835) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31914 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (0.13366) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21079 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (0.24202) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38940 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.06340) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73842 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.28561) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65227 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.19946) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75063 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.29783) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62715 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.17434) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79866 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.34586) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90481 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.45201) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22365 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.77084) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08702 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.63422) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04163 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.58883) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02098 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.56817) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06265 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-2.60984) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76947 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-3.31666) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64210 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-2.18929) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12465 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.67184) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61561 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-3.16281) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59225 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-2.13944) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60948 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.15667) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77734 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-2.32453) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76289 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-2.31008) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30833 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.85553) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29072 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-1.83791) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03681 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-1.58400) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46497 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-3.01216) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35681 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-2.90400) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.05472 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-3.60192) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76275 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-2.30995) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75269 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-2.29988) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.38472 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-2.93192) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18178 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-2.72898) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89876 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-1.44596) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.08455 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-3.63174) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.38170 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-2.92890) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74403 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-2.29123) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84871 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-2.39591) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57498 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-1.12217) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34279 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-2.88999) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61241 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-2.15960) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55655 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-2.10374) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62569 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-2.17288) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21298 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.76018) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89596 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-1.44316) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60211 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.14930) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16421 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-1.71141) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22555 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.77274) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02829 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.57548) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00562 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.55282) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68894 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.23613) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70344 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.25064) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93028 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.47748) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11501 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-1.66221) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29668 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-1.84387) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05001 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-1.59720) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28408 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-1.83127) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81289 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-1.36008) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28703 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-0.83422) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55323 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-2.10042) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48582 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-2.03302) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03118 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-1.57837) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22587 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-1.77307) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13488 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.68207) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05128 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.59848) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26381 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.81100) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26125 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-1.80844) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93153 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.47872) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61906 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.16625) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62245 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-2.16965) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17141 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-2.71861) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44019 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-1.98738) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13443 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-2.68163) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42949 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-2.97668) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82934 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-2.37653) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60055 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-2.14774) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32834 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-2.87554) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91153 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.45872) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90271 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.44990) | 1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97566 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.52286) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48999 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-2.03718) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54558 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-2.09277) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61812 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-2.16532) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12352 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-2.67072) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14031 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-2.68751) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60512 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-2.15231) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95155 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-2.49874) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72335 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-2.27055) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67881 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-1.22601) | -1 | -1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56148 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-1.10867) | 1 | 1 |
| G: -5246.08711 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33275 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-2.87994) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59363 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.14083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59345 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.14065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63185 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.17904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14154 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.68873) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44060 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.98779) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65903 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.20623) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41954 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.96673) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55290 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.10009) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41718 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.96437) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33212 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-2.87932) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69502 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-2.24222) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71102 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-2.25822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83191 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.37910) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79495 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.34215) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06179 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.60898) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97825 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.52544) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04968 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.59687) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94747 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.49467) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31189 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.85908) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18108 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.72828) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37774 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.92493) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84037 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.38756) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90029 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.44748) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90524 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.45243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60641 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.15360) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09813 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-2.64533) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11120 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-2.65839) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20924 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-2.75643) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80254 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-2.34973) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90859 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.45578) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67501 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.22220) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80390 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-2.35109) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82080 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.36800) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65002 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-2.19721) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62466 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-2.17185) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82975 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-2.37694) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15637 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-2.70356) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50493 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.05212) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30111 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.84831) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04809 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.59529) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54574 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-2.09294) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12200 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-2.66919) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.49196 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-3.03916) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78310 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-3.33029) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64046 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.18765) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56873 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.11592) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77621 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.32341) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82317 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.37037) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00260 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.54980) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94622 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.49342) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68667 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.23386) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.31944 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-2.86664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25033 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.79752) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.66854 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-3.21573) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77899 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.32618) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76299 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.31018) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43779 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (0.01502) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61831 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.16550) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57086 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-2.11805) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23472 HOMO: -6.73482 LUMO: 1.95922 factor:1 | -1 (1.21809) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51556 HOMO: -6.70489 LUMO: 2.04358 factor:1 | -1 (0.93724) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58604 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-2.13324) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79082 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.33801) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27376 HOMO: -6.40556 LUMO: 1.45581 factor:1 | -1 (0.17905) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14973 HOMO: -6.94979 LUMO: 2.16603 factor:1 | -1 (0.30308) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26799 HOMO: -6.84911 LUMO: 1.89935 factor:1 | -1 (0.18482) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57402 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.12122) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60193 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-2.14913) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75707 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.30427) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94015 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.48735) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56257 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.10976) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60485 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.15205) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51072 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-2.05792) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12592 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (0.32689) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38393 HOMO: -6.38651 LUMO: 1.53472 factor:1 | -1 (0.06887) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75052 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.29771) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88573 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.43292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96946 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.51665) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.50121 HOMO: -6.71305 LUMO: -0.49525 factor:1 | -1 (1.95160) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.81012 HOMO: -6.60692 LUMO: -0.22313 factor:1 | -1 (2.64269) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.52861 HOMO: -7.20013 LUMO: 0.55239 factor:1 | -1 (1.92420) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15328 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.70048) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17010 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.71729) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40621 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.95341) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56743 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-2.11462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76603 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.31322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79585 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.34305) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22287 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.22994) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10964 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.34316) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88766 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.43486) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78132 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.32851) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05689 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.60408) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69521 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-2.24241) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49567 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-2.04287) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42376 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.97096) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26713 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.81433) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46872 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.01591) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72498 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-2.27218) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28882 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.83602) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32305 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.87025) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60306 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.15025) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38330 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.93049) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51680 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.06399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55447 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.10166) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82778 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.37497) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88598 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.43318) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54039 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.08758) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42877 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.97596) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52700 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.07420) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13628 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-2.68348) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76301 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.31020) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64953 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-2.19672) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72184 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.26903) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33472 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.88191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24062 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.78782) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63611 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-2.18331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78651 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.33370) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46162 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-3.00882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76887 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.31606) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64742 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.19462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62078 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.16798) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49659 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.04378) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34265 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.11015) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70931 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.74350) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02096 HOMO: -6.75659 LUMO: -0.45715 factor:1 | -1 (0.43184) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65339 HOMO: -6.66135 LUMO: -0.41906 factor:1 | -1 (0.79942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96964 HOMO: -6.55794 LUMO: -0.27483 factor:1 | -1 (0.48317) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43270 HOMO: -7.07496 LUMO: -0.63403 factor:1 | -1 (0.02011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59890 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.14610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69551 HOMO: -6.53617 LUMO: -0.25579 factor:1 | -1 (0.75729) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48378 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.96902) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99338 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.54057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93485 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.48204) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59630 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.14350) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96791 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.51510) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39339 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.94059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41470 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.96190) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20672 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.75392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17949 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.72668) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06308 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.61027) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98680 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.53400) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09872 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.64592) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72889 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.27609) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03603 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.58322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67790 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.22509) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67335 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.22055) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55433 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.10153) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49662 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.04381) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52753 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.07472) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76219 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.30938) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72018 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.26737) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73375 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.28095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64007 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.18726) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36613 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.91332) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55487 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.10206) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73430 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.28149) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56952 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.11671) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55939 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.10659) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54590 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.09309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44802 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.00479) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28548 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (0.16732) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45275 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (0.00005) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74598 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.29318) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63099 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.17818) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61025 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.15745) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92429 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.47148) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78687 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.33407) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88453 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.43173) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85211 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.39930) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18566 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.73286) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67630 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-2.22350) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58664 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-2.13384) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45358 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.00077) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23604 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-2.78323) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84810 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.39529) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71596 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.26315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88799 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.43518) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92418 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.47137) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99766 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.54485) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09268 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64362 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (0.80918) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86384 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.58896) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53417 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.08136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68238 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.22957) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53470 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.08190) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62502 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.17221) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33211 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.87931) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62426 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.17145) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59049 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.13768) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74067 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.28786) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84331 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.39050) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34172 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.88891) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55884 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.10603) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40806 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.95526) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34490 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.89210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49567 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.04287) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27601 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-2.82321) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56117 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-2.10837) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79337 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.34057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75166 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.29885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80785 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.35505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39288 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.94007) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35612 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.90331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68847 HOMO: -7.23823 LUMO: -0.62858 factor:1 | -1 (0.76434) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67187 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (0.78094) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31722 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (1.13559) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63627 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.18346) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64671 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.19391) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75726 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (0.69555) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76636 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.31356) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59368 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.14087) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18573 HOMO: -6.73754 LUMO: -0.55239 factor:1 | -1 (0.26708) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07655 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (0.37625) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23269 HOMO: -6.69672 LUMO: 1.68711 factor:1 | -1 (0.22011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12374 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.32907) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40929 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (0.04351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59069 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.13788) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37626 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (0.07655) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15819 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.29462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99631 HOMO: -6.61781 LUMO: 2.13881 factor:1 | -1 (0.45650) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24130 HOMO: -6.62597 LUMO: 2.00276 factor:1 | -1 (1.21151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44135 HOMO: -7.01237 LUMO: 1.95922 factor:1 | -1 (0.01146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19136 HOMO: -7.03959 LUMO: 2.16875 factor:1 | -1 (0.26145) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29373 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (0.15908) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50983 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.05703) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30485 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.85204) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37764 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.92483) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12493 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.67212) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85842 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.40561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84242 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.38961) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52266 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.06985) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52660 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.07380) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63746 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.18466) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31710 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.13570) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31533 HOMO: -6.56067 LUMO: 1.66806 factor:1 | -1 (0.13747) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03998 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (0.41282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87807 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.57473) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97965 HOMO: -6.87360 LUMO: 1.75786 factor:1 | -1 (0.47315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72765 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (0.72516) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76441 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (0.68839) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08798 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (0.36482) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83119 HOMO: -7.09129 LUMO: 2.31569 factor:1 | -1 (0.62162) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53516 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (0.91765) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62010 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.16730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41066 HOMO: -6.78652 LUMO: 1.98371 factor:1 | -1 (0.04215) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50562 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.05282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46516 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.01235) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44834 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (0.00446) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33835 HOMO: -6.60965 LUMO: 2.20412 factor:1 | -1 (0.11445) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89865 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (0.55416) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92561 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.52719) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00722 HOMO: -6.88448 LUMO: 2.02725 factor:1 | -1 (0.44559) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57158 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.11878) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37871 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (0.07410) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51077 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.05796) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86311 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.58970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11717 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.66437) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14109 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.68828) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04678 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.59397) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21143 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.75863) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64195 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.18915) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59417 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.14136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45185 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.00095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50625 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.05344) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37700 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.07581) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60867 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.15587) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60745 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.15464) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04762 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.59481) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33440 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.88159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80650 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.35369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78898 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.33617) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99328 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.54047) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04201 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.58921) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27761 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.82480) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29493 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.15788) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41803 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.03478) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41550 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.03731) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72922 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.27641) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36099 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.09181) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56369 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.11089) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43607 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.01674) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33104 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.12177) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12968 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.67687) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04562 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.59282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15583 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.70302) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82943 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.37662) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03014 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.57734) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91308 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.46027) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14016 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.68735) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83610 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.38329) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00181 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.54901) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04271 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.58991) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97327 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.52046) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67345 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.22065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89735 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.44454) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00832 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.55551) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92056 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.46775) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06330 HOMO: -6.87360 LUMO: 1.15648 factor:1 | -1 (0.38950) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03546 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.41734) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81350 HOMO: -6.29671 LUMO: 2.43270 factor:1 | -1 (0.63930) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08978 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.36303) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76670 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.68611) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80274 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.34994) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66054 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.20773) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68018 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.22738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83246 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.37965) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08389 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.63109) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76655 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.31375) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03184 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.57903) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28336 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.16945) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81469 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.36188) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01215 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.55935) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96138 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.50857) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85550 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.40269) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73492 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.71789) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75130 HOMO: -6.47359 LUMO: 2.20412 factor:1 | -1 (0.70151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06474 HOMO: -6.90625 LUMO: 1.92384 factor:1 | -1 (0.38806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55409 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.10128) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56935 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.11655) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00797 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.55517) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19483 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.74203) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99099 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.53819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42067 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.03214) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49009 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.03728) | 1 | 1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32420 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.87139) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91099 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16974 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.71694) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98185 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.52904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14923 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.69642) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43130 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.97849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05967 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.60687) | -1 | -1 |
| G: -5246.08711 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44058 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.98777) | -1 | -1 |