乙二醇作为反应物的反应表19-15

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。

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 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: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18066 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.72785) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10672 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.65392) | 1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05388 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.60107) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99129 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.53849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29116 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.83836) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68584 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.23304) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84027 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.38746) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70329 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.25048) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92258 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.46978) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83115 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.37835) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84966 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.39685) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06925 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.61645) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97770 HOMO: -6.60965 LUMO: -0.19864 factor:1 | -1 (0.47511) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19288 HOMO: -7.29265 LUMO: 0.52246 factor:1 | -1 (0.25992) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95922 HOMO: -6.86543 LUMO: -0.59593 factor:1 | -1 (0.49359) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96504 HOMO: -7.44504 LUMO: -1.01226 factor:1 | -1 (0.48776) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08504 HOMO: -6.92530 LUMO: -0.75103 factor:1 | -1 (0.36776) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61096 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.15815) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58081 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.12800) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55651 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.10370) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84200 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.38920) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21277 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.75996) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84995 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-1.39714) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65895 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.20614) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74020 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-1.28740) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60785 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.15504) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62962 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.17681) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15206 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.69925) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06833 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.61552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07472 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.62192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79898 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-1.34617) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50703 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-1.05422) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80527 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-1.35246) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53434 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-2.08153) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50272 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-2.04992) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02121 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-2.56840) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16666 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.71385) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67162 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-2.21882) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62702 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-2.17422) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57002 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-2.11721) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26197 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-2.80917) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15612 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-2.70332) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33072 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.87791) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24449 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-1.79168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47562 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-2.02281) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34678 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.89398) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29032 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.83751) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13301 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.68020) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86864 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-1.41584) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51867 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-2.06586) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36163 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.90882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50250 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-2.04970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66132 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-1.20851) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40167 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.94886) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55332 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-1.10051) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04867 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-1.59587) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74518 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-1.29238) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09616 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-1.64335) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56254 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-1.10973) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63762 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-1.18481) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73895 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-1.28615) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32839 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.87558) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08965 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.63685) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85027 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.39747) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72911 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.27630) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95496 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.50216) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76326 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.31045) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69457 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.24176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89906 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.44626) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69824 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.24544) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97010 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-2.51730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48833 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.03552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50201 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-2.04921) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99990 HOMO: -7.18381 LUMO: -0.92791 factor:1 | -1 (0.45291) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34113 HOMO: -6.49264 LUMO: -0.44627 factor:1 | -1 (0.11168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18148 HOMO: -7.32803 LUMO: 0.41361 factor:1 | -1 (0.27132) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44240 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.98960) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38319 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.93038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10667 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.65386) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88412 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-1.43132) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13036 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.67755) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90328 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-1.45048) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03826 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.58545) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13734 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-0.68453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45728 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-2.00447) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24087 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.78806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78724 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-2.33444) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44999 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.99718) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31448 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.86168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15932 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.70652) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72712 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.27432) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84217 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.38937) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58968 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.13687) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51980 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.06699) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65085 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.19804) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89927 HOMO: -6.71305 LUMO: -0.61226 factor:1 | -1 (0.55353) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73973 HOMO: -7.06408 LUMO: 0.80001 factor:1 | -1 (0.71307) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90061 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (0.55220) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59031 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (0.86249) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98542 HOMO: -6.85455 LUMO: 0.84900 factor:1 | -1 (0.46738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85823 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.40542) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87145 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-0.41865) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63455 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.18174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19124 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.73844) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19448 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.74167) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71892 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.26612) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81248 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.35967) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31012 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.85731) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86115 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-2.40834) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31842 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-1.86561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20106 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-1.74825) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72099 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.26819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87846 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.42566) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24074 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.78793) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67765 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.22485) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.46373 HOMO: -6.37563 LUMO: -0.48164 factor:1 | -1 (0.98908) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84694 HOMO: -6.64774 LUMO: -0.71838 factor:1 | -1 (0.60586) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68153 HOMO: -7.17020 LUMO: 0.45987 factor:1 | -1 (0.77128) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79325 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.34044) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41242 HOMO: -6.77019 LUMO: -1.03131 factor:1 | -1 (0.04038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60096 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-1.14816) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65128 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.19847) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83452 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-1.38171) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99071 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.53791) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41658 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.96377) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53373 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.08093) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85643 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.40363) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.57627 HOMO: -6.82734 LUMO: -0.68301 factor:1 | -1 (0.87653) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54076 HOMO: -6.48175 LUMO: -2.19052 factor:1 | -1 (0.91204) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99130 HOMO: -6.65863 LUMO: -0.77008 factor:1 | -1 (0.46151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93740 HOMO: -6.44094 LUMO: -2.20956 factor:1 | -1 (0.51541) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92501 HOMO: -6.59876 LUMO: -0.57688 factor:1 | -1 (0.52779) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13566 HOMO: -6.78380 LUMO: -0.77008 factor:1 | -1 (0.31715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66629 HOMO: -7.30354 LUMO: 0.25034 factor:1 | -1 (0.78652) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35929 HOMO: -6.59332 LUMO: -0.53334 factor:1 | -1 (1.09352) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25243 HOMO: -6.64230 LUMO: -0.55783 factor:1 | -1 (1.20038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93070 HOMO: -7.26544 LUMO: 0.20409 factor:1 | -1 (0.52210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79149 HOMO: -6.61237 LUMO: -0.65307 factor:1 | -1 (0.66132) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84969 HOMO: -6.72393 LUMO: -0.65307 factor:1 | -1 (0.60311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73258 HOMO: -6.29671 LUMO: -0.39729 factor:1 | -1 (0.72023) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15091 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.69810) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12285 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.67004) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97115 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.51834) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17613 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-1.72332) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94902 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-2.49621) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34767 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.89486) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43728 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.98447) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11168 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.65887) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67250 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.21970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43848 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.98568) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49263 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.03983) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54684 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.09403) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67849 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.22568) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52142 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.06862) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80140 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.34860) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70024 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.24743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83192 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.37911) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52029 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.06748) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34105 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (0.11176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45071 HOMO: -6.54434 LUMO: -0.42994 factor:1 | -1 (0.00210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78794 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-0.33514) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68742 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.23462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91456 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.46175) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84590 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.39310) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05962 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.60681) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80408 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.35127) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23987 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.78706) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05562 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.60281) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21969 HOMO: -6.44638 LUMO: -0.45171 factor:1 | -1 (0.23312) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10208 HOMO: -7.07496 LUMO: 0.50341 factor:1 | -1 (0.35073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20701 HOMO: -6.79468 LUMO: 0.11429 factor:1 | -1 (0.24580) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64979 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.19698) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78353 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.33073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73137 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.27856) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60671 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.15391) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81445 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.36164) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39335 HOMO: -6.64502 LUMO: 1.79323 factor:1 | -1 (0.05946) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53472 HOMO: -6.51168 LUMO: 1.60275 factor:1 | -1 (0.91808) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35706 HOMO: -6.56067 LUMO: 1.63268 factor:1 | -1 (1.09575) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93816 HOMO: -6.56883 LUMO: 1.70615 factor:1 | -1 (0.51465) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68569 HOMO: -6.77836 LUMO: 1.77962 factor:1 | -1 (0.76712) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64368 HOMO: -6.38923 LUMO: 1.85854 factor:1 | -1 (0.80913) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04044 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.58763) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64696 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-0.19415) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29986 HOMO: -6.87087 LUMO: 1.79051 factor:1 | -1 (1.15295) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.61265 HOMO: -6.56339 LUMO: 2.37828 factor:1 | -1 (0.84015) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45246 HOMO: -6.30488 LUMO: 2.51705 factor:1 | -1 (1.00034) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29674 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.84393) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31354 HOMO: -6.51168 LUMO: 2.03541 factor:1 | -1 (0.13927) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62323 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.17042) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78274 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.32993) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26678 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.81397) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67155 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.21874) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47361 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-2.02080) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97258 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-2.51977) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41486 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.96205) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84614 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.39333) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61654 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.16373) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66369 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.21089) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56328 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-0.11048) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53762 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-0.08482) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53575 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.08294) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58752 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.13471) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37274 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.91994) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51220 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.05939) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98919 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.53638) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74486 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-1.29205) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64536 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-2.19256) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26532 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-2.81251) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59260 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-2.13979) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83609 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-2.38328) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62317 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.17036) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63917 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.18636) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39222 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.93942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54966 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-2.09685) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50484 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-2.05204) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41200 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.95919) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92388 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.47107) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57671 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-2.12390) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66000 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-2.20720) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42986 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.97705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62543 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.17262) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32967 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.87686) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44734 HOMO: -6.40828 LUMO: 2.10072 factor:1 | -1 (0.00547) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23601 HOMO: -6.06542 LUMO: 1.92112 factor:1 | -1 (0.21679) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59844 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.14564) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37090 HOMO: -6.37019 LUMO: 1.92929 factor:1 | -1 (0.08191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50024 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.04743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63207 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.17926) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49715 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.04435) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24314 HOMO: -6.49536 LUMO: 1.75241 factor:1 | -1 (0.20966) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30214 HOMO: -6.34297 LUMO: 1.86398 factor:1 | -1 (0.15067) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38075 HOMO: -6.53073 LUMO: 1.84493 factor:1 | -1 (0.07206) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95387 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.50106) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23222 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.77942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33816 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.88535) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29132 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.83852) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40801 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.95520) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31552 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.86271) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23875 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-0.78595) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07535 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-0.62254) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29380 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.84100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42379 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-0.97098) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29187 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-0.83906) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30063 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-0.84783) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10523 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.65242) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16694 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.71414) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03554 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.58273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27685 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.82404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27927 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.82646) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16993 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.71713) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22147 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.76867) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11491 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.66211) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32588 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.87308) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33935 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-0.88655) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27737 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.82456) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08101 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.62820) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35255 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.89974) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80380 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.35099) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21978 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-1.76697) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16122 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-1.70841) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42559 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.97278) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18664 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.73384) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84664 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.39383) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02064 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.56784) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98888 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-2.53607) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12742 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.67462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58460 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-2.13179) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54240 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-2.08959) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52938 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.07657) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52102 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.06822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31392 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (0.13889) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47996 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.02716) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34973 HOMO: -6.88448 LUMO: 0.82723 factor:1 | -1 (0.10308) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96324 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.51043) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89611 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.44330) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72955 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.27674) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84813 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.39533) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90816 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.45536) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90307 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.45027) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82280 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.36999) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89001 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.43721) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07627 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.62347) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04030 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.58749) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89747 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.44466) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44074 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.98794) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01235 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.55955) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54309 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.09029) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28453 HOMO: -6.75659 LUMO: -0.41361 factor:1 | -1 (0.16828) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53180 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.07899) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22690 HOMO: -6.89264 LUMO: -0.90886 factor:1 | -1 (0.22591) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45806 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.00525) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03244 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.57963) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26542 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.81261) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99206 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.46074) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04221 HOMO: -6.41100 LUMO: 0.79185 factor:1 | -1 (0.41059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39759 HOMO: -6.39195 LUMO: 0.26123 factor:1 | -1 (0.05521) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99048 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.46232) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19022 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.26259) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61466 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-0.16185) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30614 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (0.14667) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39417 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (0.05864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64228 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.18947) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80089 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.34809) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64984 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.19704) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81877 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.36597) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44772 HOMO: -6.92802 LUMO: -0.72927 factor:1 | -1 (0.00509) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90751 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.45470) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04581 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.59301) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78717 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-1.33436) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87223 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.41943) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07899 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-1.62618) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54222 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.08942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50372 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.05091) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51673 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.06392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29242 HOMO: -6.90081 LUMO: 1.25444 factor:1 | -1 (0.16038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20382 HOMO: -7.00965 LUMO: -1.05036 factor:1 | -1 (0.24898) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19120 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.26161) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94930 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.49650) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90272 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.44991) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82302 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.37021) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80176 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.34896) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00430 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.55149) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37271 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.91991) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44025 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.98745) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53764 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-1.08484) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58439 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-1.13159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63582 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-1.18302) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93374 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-0.48093) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69858 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.24577) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79096 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.33816) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90403 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.45122) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72035 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.26754) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81861 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.36580) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65597 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.20316) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65757 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.20477) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73959 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.28678) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09197 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-1.63916) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08029 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-1.62749) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10957 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-1.65677) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07224 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.61943) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04410 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.59129) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01945 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.56664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99251 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-1.53970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92998 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.47717) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07471 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.62191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70840 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-0.25560) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91265 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.45985) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84895 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.39614) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01273 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.55993) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89777 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.44496) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73393 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.28112) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75755 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.30474) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83246 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-0.37965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00827 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.55547) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66094 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.20813) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70162 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.24881) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60015 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.14734) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61313 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.16032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79513 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.34232) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44667 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.99387) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00528 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.55247) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37380 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.92100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31639 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.86358) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78756 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.33475) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12452 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.67171) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68201 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.22920) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98661 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.53381) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73472 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.28191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96732 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.51451) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41740 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.96459) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31701 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.86421) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39984 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.94704) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29777 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.84497) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51563 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-1.06282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47269 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-1.01988) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68252 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.22971) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63163 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.17882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63354 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-1.18073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75947 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-1.30666) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93701 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.48420) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00607 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.55326) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21845 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.76565) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00735 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.55454) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84366 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-1.39086) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74665 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.29385) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73152 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.27872) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76725 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.31445) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69685 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-2.24404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62738 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-2.17457) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25122 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-2.79842) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37164 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.91884) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22057 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-1.76776) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92170 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-2.46889) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88520 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-2.43240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43213 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-1.97933) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59002 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-1.13722) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92066 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-2.46786) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98317 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-2.53036) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77981 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-2.32701) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05160 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-2.59880) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93498 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-1.48218) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84864 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-1.39584) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09912 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.64632) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22125 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-1.76844) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23619 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.78338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97942 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.52661) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87931 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.42650) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88524 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.43243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98886 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.53606) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81400 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.36120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14454 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.69173) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51475 HOMO: -6.28583 LUMO: 0.40545 factor:1 | -1 (0.93806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68789 HOMO: -6.70761 LUMO: 0.41906 factor:1 | -1 (0.76491) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60221 HOMO: -6.76203 LUMO: -0.60954 factor:1 | -1 (0.85060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08347 HOMO: -6.85999 LUMO: -0.75103 factor:1 | -1 (0.36934) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00376 HOMO: -7.19741 LUMO: -1.00954 factor:1 | -1 (0.44904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86999 HOMO: -6.58243 LUMO: -0.33470 factor:1 | -1 (0.58281) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10178 HOMO: -7.22190 LUMO: 0.49253 factor:1 | -1 (0.35103) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82619 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.37339) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63413 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-1.18133) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56137 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-1.10856) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17294 HOMO: -6.33753 LUMO: -0.48436 factor:1 | -1 (0.27987) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10553 HOMO: -7.15932 LUMO: 0.55511 factor:1 | -1 (0.34727) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39433 HOMO: -6.57427 LUMO: 2.01908 factor:1 | -1 (0.05848) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26771 HOMO: -6.75659 LUMO: 2.22045 factor:1 | -1 (0.18509) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09767 HOMO: -6.73482 LUMO: 2.20956 factor:1 | -1 (0.35514) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87634 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-1.42354) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18980 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.73699) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08865 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.63585) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37016 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.91735) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85965 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-2.40685) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.66291 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-3.21010) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80338 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-2.35057) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01596 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-2.56315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97751 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.52471) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97806 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.52525) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48483 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.03202) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69588 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.24307) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50344 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.05063) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63901 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.18621) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96280 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.51000) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76702 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.31421) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59979 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-1.14699) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88524 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-1.43243) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31709 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-1.86428) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30549 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-1.85269) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84761 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-1.39480) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95153 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.49872) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79063 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-1.33782) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79512 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-1.34231) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26763 HOMO: -6.15249 LUMO: 1.98643 factor:1 | -1 (0.18517) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22358 HOMO: -6.19331 LUMO: 2.14154 factor:1 | -1 (0.22923) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43272 HOMO: -6.05998 LUMO: 2.12521 factor:1 | -1 (0.02008) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43700 HOMO: -6.67223 LUMO: 1.91840 factor:1 | -1 (0.01581) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36543 HOMO: -6.79196 LUMO: 2.18507 factor:1 | -1 (0.08738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43765 HOMO: -6.93346 LUMO: 1.78235 factor:1 | -1 (0.01516) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49716 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.04435) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46102 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-0.00822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52549 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.07268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24841 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.79561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26833 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.81553) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30844 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.85563) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91229 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-1.45948) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78611 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-1.33330) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23958 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-2.78677) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50318 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-2.05038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54561 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-2.09280) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56057 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-2.10777) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97973 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.52692) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25641 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.80361) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14675 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.69394) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91940 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.46659) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37655 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.92374) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20545 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.75264) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09540 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.64260) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16686 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.71405) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41184 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.95904) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77466 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.32186) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11573 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.66292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09238 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.63958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99521 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.54240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04773 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.59492) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38632 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.93351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94743 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.49462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93350 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.48069) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60605 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.15325) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50869 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.05588) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50355 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.05074) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71022 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.25741) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30022 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-0.84742) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93857 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-2.48576) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14911 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.69630) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31330 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-1.86050) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52697 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-2.07416) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08742 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-1.63462) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22644 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.77364) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15814 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.70534) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32411 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.87130) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01093 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.55812) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05724 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-1.60444) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34038 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.88757) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93158 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.47878) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11967 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.66686) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97757 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.52476) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36294 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.91013) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45864 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-2.00583) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52893 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-2.07612) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52054 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-2.06774) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40335 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-0.95055) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30167 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.84886) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.29196 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-2.83915) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30382 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-2.85102) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05560 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-2.60280) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09294 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-2.64013) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81346 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.36065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94429 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.49148) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97330 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.52049) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85389 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.40109) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69324 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.24043) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79860 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.34579) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88219 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.42939) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92998 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.47717) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81718 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-2.36437) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03980 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.58700) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14584 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-2.69303) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.55833 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-3.10553) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89121 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.43840) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80680 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.35399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35505 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.90225) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01182 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-2.55901) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14679 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-2.69398) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86684 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-2.41403) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89723 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-2.44443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66012 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.20731) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72777 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.27496) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47535 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-2.02254) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88252 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.42971) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65324 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-1.20043) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48727 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-2.03446) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56463 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-2.11182) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88995 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.43714) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79925 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-1.34645) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96072 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-1.50792) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70418 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.25137) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73797 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.28517) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73463 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.28182) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78453 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.33173) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79313 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.34032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78954 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.33673) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78742 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.33461) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68439 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.23159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55900 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.10620) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82578 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.37298) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59427 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.14146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73101 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.27820) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87144 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.41864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86592 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.41311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73650 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.28370) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81506 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-1.36226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68102 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.22821) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90094 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.44814) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69351 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.24070) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81789 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.36509) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39499 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.94219) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32215 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.86934) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23208 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.77927) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42718 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.97438) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32062 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.86782) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41116 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.95835) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44819 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.99538) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33352 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-1.88071) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36691 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.91410) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96847 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-2.51567) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84722 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.39441) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58629 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-2.13348) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62444 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-2.17163) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71000 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.25719) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48896 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.03616) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94850 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-2.49569) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52989 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.07708) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10162 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-2.64881) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52637 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-2.07356) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07142 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.61861) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79718 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-1.34438) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08731 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.63451) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92252 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.46971) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77446 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.32166) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77060 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-1.31779) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69454 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-1.24174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97392 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-1.52112) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77416 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-1.32136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59155 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.13874) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31230 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-1.85949) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67459 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-2.22178) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57462 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.12182) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33135 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.87855) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21645 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-2.76364) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56626 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-2.11345) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61080 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-2.15800) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17731 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.72450) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34769 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.89488) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50649 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-3.05369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.18289 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-3.73008) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78378 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-3.33097) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91802 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-2.46522) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80463 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-2.35183) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50307 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-3.05026) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80558 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-2.35278) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79340 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.34060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66888 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.21608) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74172 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-2.28891) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87319 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-1.42038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02809 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-2.57529) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68679 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.23398) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59483 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-2.14203) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70039 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.24759) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65589 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-2.20309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70985 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-2.25705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76235 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-2.30954) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69900 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-2.24619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37833 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-2.92552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55962 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-2.10681) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46615 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-2.01334) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33566 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-2.88286) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65611 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-2.20331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70136 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-2.24856) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65102 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-2.19822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70436 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-2.25155) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35229 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-2.89948) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34114 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.88833) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06325 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-2.61044) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44601 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-1.99321) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49956 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-2.04676) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28479 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-1.83198) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21468 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-2.76187) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48593 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-2.03313) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32603 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-2.87322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.83526 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-3.38246) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09318 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-2.64038) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98681 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-2.53401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.57052 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-3.11772) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.74239 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-3.28958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10045 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-2.64764) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69730 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-3.24450) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50566 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-2.05285) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14649 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-2.69368) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17993 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-2.72713) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49859 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-2.04578) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33112 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-2.87831) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64079 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-2.18799) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91454 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-2.46173) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11343 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-2.66062) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43189 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.97908) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08744 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-2.63463) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.62685 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-3.17404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69736 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-3.24455) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13941 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-2.68661) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25950 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-2.80669) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65791 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-2.20510) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84987 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.39707) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75322 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.30041) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17141 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-2.71861) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77600 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.32319) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75491 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.30210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70995 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.25715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83284 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.38003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76582 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.31301) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84324 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-2.39044) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61935 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-2.16654) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64161 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-2.18880) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68349 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-2.23068) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78106 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.32825) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.52701 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-3.07421) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00654 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-2.55373) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98702 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.53421) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99455 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-1.54174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75366 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-2.30086) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98168 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.52887) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23261 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-2.77981) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44843 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-2.99562) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22654 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-2.77374) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06657 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-2.61376) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01405 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-2.56124) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24205 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.78924) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46833 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-1.01553) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26455 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.81174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92338 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-2.47058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78115 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-2.32834) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85851 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-2.40570) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67861 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.22580) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85545 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.40265) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81638 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.36357) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62293 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.17013) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98296 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.53015) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39431 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.94151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45752 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-2.00472) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72224 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-1.26944) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75378 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-1.30098) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71182 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-1.25902) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84006 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-2.38725) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76839 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-2.31558) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46875 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-3.01595) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76362 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-2.31082) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62506 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-2.17226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52776 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-1.07496) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45848 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-1.00568) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48463 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-1.03183) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27651 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.82371) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26563 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-1.81282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12280 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-1.66999) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15052 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.69772) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77897 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-2.32617) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64384 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-2.19103) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96151 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-2.50870) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76640 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-2.31359) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53514 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-1.08233) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46771 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-1.01490) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66459 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.21179) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70086 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.24806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40557 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-2.95276) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22754 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.77474) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25916 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.80636) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19094 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.73814) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72460 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-2.27180) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14924 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-2.69643) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55453 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-2.10173) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51989 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-2.06709) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52411 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-2.07130) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64381 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-2.19101) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25375 HOMO: -6.55250 LUMO: -0.49797 factor:1 | -1 (0.19905) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48465 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-2.03185) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18760 HOMO: -7.45320 LUMO: 0.08436 factor:1 | -1 (0.26520) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56611 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.11331) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83500 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-2.38219) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39677 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.94396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46118 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-1.00837) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52774 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-1.07493) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41896 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-1.96616) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92935 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.47654) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73973 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-2.28693) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96720 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-1.51440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89210 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-1.43929) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49072 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (0.96209) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73587 HOMO: -5.98378 LUMO: 0.78641 factor:1 | -1 (0.71694) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13966 HOMO: -6.11440 LUMO: 0.71294 factor:1 | -1 (0.31315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83845 HOMO: -6.45182 LUMO: 0.63947 factor:1 | -1 (0.61435) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23406 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (1.21874) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33719 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (1.11561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08085 HOMO: -6.66679 LUMO: 0.48708 factor:1 | -1 (0.37195) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51418 HOMO: -6.81917 LUMO: 0.31021 factor:1 | -1 (0.93863) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68732 HOMO: -6.28583 LUMO: 0.44899 factor:1 | -1 (0.76548) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80019 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.34738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79480 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.34199) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50682 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.05401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63036 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-0.17755) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30325 HOMO: -6.04909 LUMO: -0.59865 factor:1 | -1 (0.14955) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46551 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.01271) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65169 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.19889) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49520 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.04240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44894 HOMO: -6.80557 LUMO: -0.57416 factor:1 | -1 (0.00386) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86116 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-1.40835) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68135 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-1.22854) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79316 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-1.34035) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79264 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-1.33983) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62422 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-2.17141) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98473 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.53192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92470 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-1.47189) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91749 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.46468) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92399 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.47118) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95879 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.50599) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89675 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.44394) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65740 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.20459) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68181 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.22900) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41476 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.96195) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67269 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.21989) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40507 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.95226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32676 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (0.12604) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46143 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.00863) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69227 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.23946) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64380 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-0.19100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38821 HOMO: -6.81917 LUMO: 2.41365 factor:1 | -1 (0.06460) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73246 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.27965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40652 HOMO: -7.04775 LUMO: 2.31025 factor:1 | -1 (0.04629) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44119 HOMO: -6.64774 LUMO: 2.20140 factor:1 | -1 (0.01162) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12404 HOMO: -6.72393 LUMO: 2.28304 factor:1 | -1 (0.32877) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20420 HOMO: -6.35114 LUMO: 1.84765 factor:1 | -1 (0.24860) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58236 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.12955) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32018 HOMO: -6.34297 LUMO: 1.55921 factor:1 | -1 (0.13263) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19280 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (0.26000) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44728 HOMO: -6.50896 LUMO: 2.02725 factor:1 | -1 (0.00552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22905 HOMO: -6.28583 LUMO: 2.00548 factor:1 | -1 (0.22376) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60075 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.14795) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71553 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.26273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39803 HOMO: -6.84911 LUMO: 2.24766 factor:1 | -1 (0.05478) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95069 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.49789) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71831 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.26550) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70802 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-0.25522) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52502 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.07221) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05393 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.60113) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29198 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.83917) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35825 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (0.09456) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54764 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.09483) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57542 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.12261) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33855 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (0.11426) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33387 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (0.11894) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40339 HOMO: -6.70489 LUMO: 2.20956 factor:1 | -1 (0.04942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85060 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.39779) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67375 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-1.22095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34843 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.89563) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19340 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-2.74059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09155 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-2.63874) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68613 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-2.23332) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45472 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.00191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68056 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.22775) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41675 HOMO: -6.93618 LUMO: 1.75513 factor:1 | -1 (0.03606) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66565 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.21285) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55343 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.10063) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51188 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.05908) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30140 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (0.15140) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31093 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (0.14188) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31388 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-0.86108) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35824 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-0.90543) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64192 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.18911) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38945 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-0.93664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16256 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-0.70975) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50521 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-1.05240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15598 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.70317) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25565 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-0.80284) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92832 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.47552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12985 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.67705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65563 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.20282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52289 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.07009) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25305 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-2.80024) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40816 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-1.95536) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52313 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-2.07032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61222 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-2.15941) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65282 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-2.20001) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66831 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-1.21551) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49136 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-1.03855) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62105 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.16824) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91606 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-2.46326) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64842 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-1.19561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73724 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-1.28443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93860 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.48580) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67051 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-2.21770) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52930 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.07649) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49199 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.03918) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12832 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.67551) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29734 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.84453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49944 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-1.04663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33505 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-0.88225) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60245 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (0.85036) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63763 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.81517) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26488 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (0.18792) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19326 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.25954) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49553 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.04272) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21286 HOMO: -6.68312 LUMO: 2.30208 factor:1 | -1 (0.23995) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02485 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (0.42795) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38029 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (0.07252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55430 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-1.10149) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52053 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-1.06772) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.38185 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (1.07096) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.28046 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (1.17235) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09451 HOMO: -6.61781 LUMO: 2.11432 factor:1 | -1 (0.35829) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98357 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (0.46923) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57823 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-2.12543) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83052 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.37771) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70439 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-1.25159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29228 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.83947) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40363 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.95082) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37212 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.91931) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36608 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (0.08672) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17686 HOMO: -6.61781 LUMO: 2.24494 factor:1 | -1 (0.27595) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24932 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (0.20349) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02235 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.43046) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45045 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.99764) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52464 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-1.07183) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77449 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.32168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71759 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.26479) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53770 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.08489) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48107 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.02826) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31151 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.85870) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13841 HOMO: -6.43277 LUMO: 1.80956 factor:1 | -1 (0.31440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05775 HOMO: -6.71577 LUMO: -0.81090 factor:1 | -1 (0.39505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19242 HOMO: -7.14027 LUMO: -0.68028 factor:1 | -1 (0.26039) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70437 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-1.25156) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36648 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.91368) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41565 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.96285) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93264 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.47984) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72330 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-2.27049) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81561 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-1.36280) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91757 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.46476) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12019 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.66739) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97796 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-0.52515) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97521 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-0.52240) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17543 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-0.72263) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44970 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (0.00310) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57273 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.11992) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52296 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-0.07015) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86919 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.41639) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36023 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.09257) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22135 HOMO: -6.39195 LUMO: 1.84221 factor:1 | -1 (0.23146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29299 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (0.15981) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19090 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (0.26191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92021 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.46740) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85425 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.40144) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80384 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-2.35104) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89196 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-1.43916) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02081 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-1.56800) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71422 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.26141) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65737 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.20457) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72731 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.27450) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67506 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.22225) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27445 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-1.82164) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16239 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-1.70958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20410 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.75130) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12092 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.66811) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08282 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-1.63002) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13869 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.68588) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01719 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-1.56438) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63187 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-2.17906) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68006 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-2.22725) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58212 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-2.12932) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57167 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-2.11887) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07343 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.62063) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72973 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.27692) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26436 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.81155) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26912 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.81631) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89074 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.43793) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09679 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.64398) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28841 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-0.83561) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11559 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-0.66279) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33579 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-0.88298) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68085 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.77196) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52735 HOMO: -6.79196 LUMO: 2.06534 factor:1 | -1 (0.92546) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16415 HOMO: -6.70216 LUMO: 1.83405 factor:1 | -1 (0.28866) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15710 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.29571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83930 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-2.38649) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05743 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.60463) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89509 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-1.44229) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72660 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.27379) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86510 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.41230) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82679 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-1.37398) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74956 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-1.29676) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40415 HOMO: -6.97972 LUMO: 2.11432 factor:1 | -1 (0.04865) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29827 HOMO: -6.17154 LUMO: 1.98099 factor:1 | -1 (0.15453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43759 HOMO: -6.74026 LUMO: 2.21501 factor:1 | -1 (0.01521) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56628 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.11347) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76010 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.30729) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75868 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.30587) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74595 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.29314) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48820 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.03539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81708 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.36427) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71623 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.26342) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94892 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.49611) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91920 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.46639) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61722 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.16441) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54456 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.09176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58214 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.12934) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62217 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.16936) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41448 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.96168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41726 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.96445) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51585 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.06304) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32069 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.86788) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26466 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.81185) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34251 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.88970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27241 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.81961) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95887 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.50607) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19109 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-2.73828) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51241 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-2.05960) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42226 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.96945) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51518 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-2.06238) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83574 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-1.38294) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58338 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.13058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63250 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.17970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58602 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.13322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58021 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.12740) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39142 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.06139) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40646 HOMO: -6.35930 LUMO: 1.78507 factor:1 | -1 (0.04634) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88807 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-1.43526) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44474 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.99194) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31407 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.86127) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42390 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-0.97109) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45119 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.99839) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42956 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.97675) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56845 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.11564) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53081 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.07801) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81852 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.36571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69650 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.24370) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00337 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-1.55056) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82755 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.37475) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64837 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.19556) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75833 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-1.30552) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53645 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-1.08364) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85961 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.40680) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98323 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-1.53042) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61149 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-2.15868) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99381 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-1.54101) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05536 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-2.60255) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.23755 HOMO: -6.79468 LUMO: 1.96466 factor:1 | -1 (2.21525) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.63100 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (1.82180) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.52681 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (1.92599) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.45174 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (2.00107) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.14346 HOMO: -6.56883 LUMO: 1.64085 factor:1 | -1 (2.30935) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.44602 HOMO: -7.19197 LUMO: 2.66127 factor:1 | -1 (2.00679) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69676 HOMO: -6.48175 LUMO: 2.40004 factor:1 | -1 (0.75604) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93405 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (0.51876) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47202 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.01921) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.77678 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (2.67602) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.88952 HOMO: -6.59332 LUMO: 1.81772 factor:1 | -1 (2.56329) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.04544 HOMO: -6.68312 LUMO: 2.41909 factor:1 | -1 (2.40736) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.39217 HOMO: -5.87494 LUMO: 2.18235 factor:1 | -1 (2.06064) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.55963 HOMO: -6.30488 LUMO: 2.04902 factor:1 | -1 (1.89318) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.40364 HOMO: -6.65046 LUMO: 2.05446 factor:1 | -1 (1.04916) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.00222 HOMO: -6.55794 LUMO: 2.06807 factor:1 | -1 (1.45058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48048 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.02767) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45506 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.00226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71455 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.26175) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57991 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.12710) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43553 HOMO: -7.15115 LUMO: 2.07351 factor:1 | -1 (0.01728) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69335 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.24055) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83564 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.38284) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69273 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.23992) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02068 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.56787) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40138 HOMO: -6.78380 LUMO: 2.43542 factor:1 | -1 (0.05143) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67754 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.22474) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62821 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.17540) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00305 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.55024) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51540 HOMO: -6.17426 LUMO: 1.45853 factor:1 | -1 (0.93741) | -1 | -1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64471 HOMO: -7.21374 LUMO: 2.33474 factor:1 | -1 (0.80810) | 1 | 1 |
| G: -5246.08711 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72977 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.72303) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72172 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (0.73109) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.33195 HOMO: -7.19469 LUMO: 1.60819 factor:1 | -1 (2.12086) | 1 | 1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.86366 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (1.58914) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.79615 HOMO: -6.70489 LUMO: 0.74559 factor:1 | -1 (1.65666) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.96900 HOMO: -6.72393 LUMO: 0.88981 factor:1 | -1 (1.48381) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.84597 HOMO: -4.54430 LUMO: -0.90614 factor:1 | -1 (1.60683) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34445 HOMO: -6.83006 LUMO: 0.47348 factor:1 | -1 (0.10836) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51523 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.06242) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36652 HOMO: -6.62053 LUMO: 0.74559 factor:1 | -1 (0.08629) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34418 HOMO: -6.79196 LUMO: 1.80139 factor:1 | -1 (0.10863) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33969 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (0.11312) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42508 HOMO: -6.74026 LUMO: 0.95784 factor:1 | -1 (0.02773) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11845 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.66564) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22751 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.77470) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09323 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.64042) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29538 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.84257) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32681 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-0.87400) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21462 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-0.76181) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33094 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.87814) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50015 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.04734) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38869 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.93588) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92723 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.47442) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89623 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.44343) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81222 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-2.35942) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74701 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.29420) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82263 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.36982) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75512 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.30231) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86113 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.40833) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01113 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.55832) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33571 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-0.88290) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08296 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-1.63015) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12903 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-1.67622) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95911 HOMO: -7.09129 LUMO: -0.66668 factor:1 | -1 (0.49370) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32908 HOMO: -6.96884 LUMO: -0.31021 factor:1 | -1 (0.12373) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45549 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.00269) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39666 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.94385) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30030 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.84750) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39590 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.94309) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48496 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.03216) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39495 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.94214) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81933 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.36653) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06569 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.61288) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28724 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-0.83444) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72110 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.26830) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66701 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.21420) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65936 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.20655) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51044 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.05763) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32089 HOMO: -6.47903 LUMO: 0.24762 factor:1 | -1 (0.13192) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38655 HOMO: -6.15249 LUMO: 0.32109 factor:1 | -1 (0.06626) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18499 HOMO: -6.84366 LUMO: 0.29116 factor:1 | -1 (0.26781) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48551 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.03270) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64842 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.19561) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.91983) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17120 HOMO: -7.24095 LUMO: 0.15238 factor:1 | -1 (0.28161) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08001 HOMO: -7.06952 LUMO: -0.34558 factor:1 | -1 (0.37280) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33019 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (0.12261) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19596 HOMO: -6.37291 LUMO: -0.69117 factor:1 | -1 (0.25685) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87319 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.42038) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52036 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.06756) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88989 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-1.43709) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71109 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.25828) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55455 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.10174) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49409 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.04128) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49458 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.04177) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44478 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (0.00803) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10077 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-2.64797) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38569 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.93288) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42770 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.97489) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55352 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-2.10072) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24444 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.79163) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20708 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.75427) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04297 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.59016) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31737 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.86456) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78644 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.33364) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29943 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.84663) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19396 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.74116) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83428 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.38148) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98473 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.53193) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26526 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.81245) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15546 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.70265) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99031 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.53751) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33328 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.88048) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.76001 HOMO: -6.08174 LUMO: -0.82995 factor:1 | -1 (1.69279) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.89977 HOMO: -6.42189 LUMO: -0.84355 factor:1 | -1 (1.55304) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.46387 HOMO: -6.53890 LUMO: 0.60409 factor:1 | -1 (1.98893) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.03253 HOMO: -6.62869 LUMO: 0.43810 factor:1 | -1 (1.42027) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25496 HOMO: -6.68312 LUMO: 0.64491 factor:1 | -1 (1.19785) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.98244 HOMO: -6.42189 LUMO: 1.51295 factor:1 | -1 (1.47037) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11127 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.65846) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00863 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.55582) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08765 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.63484) | 1 | 1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91853 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.46572) | 1 | 1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17377 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.72097) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91659 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.46378) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78393 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.33113) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08995 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.63715) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60402 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.15121) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97861 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.52581) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54290 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.09010) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04599 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.59318) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79674 HOMO: -6.94162 LUMO: -0.08980 factor:1 | -1 (0.65607) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94586 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.50695) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51758 HOMO: -6.75114 LUMO: 0.04626 factor:1 | -1 (0.93523) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46709 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.01429) | 1 | 1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40083 HOMO: -7.36612 LUMO: 0.63675 factor:1 | -1 (0.05197) | 1 | 1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85695 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.40414) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42105 HOMO: -6.89264 LUMO: -0.54967 factor:1 | -1 (0.03176) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94860 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.49579) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51027 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.05746) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56417 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.11137) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51160 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.05880) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60875 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.15594) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37746 HOMO: -6.18515 LUMO: -0.85988 factor:1 | -1 (0.07535) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91279 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.45998) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36946 HOMO: -6.37563 LUMO: -1.74697 factor:1 | -1 (0.08335) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51025 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.05744) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62095 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.16814) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61213 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.15932) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75529 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.30248) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37430 HOMO: -6.05453 LUMO: -0.83539 factor:1 | -1 (0.07850) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24573 HOMO: -7.35252 LUMO: -0.45715 factor:1 | -1 (0.20708) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27073 HOMO: -6.41644 LUMO: -0.97417 factor:1 | -1 (0.18207) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17207 HOMO: -6.78924 LUMO: 0.36735 factor:1 | -1 (0.28074) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21348 HOMO: -6.74298 LUMO: 0.51974 factor:1 | -1 (0.23932) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05244 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.59963) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33424 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.88143) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04871 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.59590) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21151 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-0.75871) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33772 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.88491) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02405 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.57125) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54401 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-1.09120) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85199 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-1.39918) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59851 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-1.14571) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82486 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-1.37205) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81574 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.36294) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37696 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.92415) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52020 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-1.06739) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22317 HOMO: -6.39740 LUMO: 0.83267 factor:1 | -1 (0.22964) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95470 HOMO: -6.44094 LUMO: 0.65579 factor:1 | -1 (0.49810) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31035 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (0.14245) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16148 HOMO: -7.10217 LUMO: 0.49797 factor:1 | -1 (0.29133) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64703 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-1.19423) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73792 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.28511) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99675 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-1.54395) | -1 | -1 |
| G: -5246.08711 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98502 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-1.53222) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83904 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-1.38623) | 1 | 1 |
| G: -5246.08711 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85917 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-1.40637) | -1 | -1 |
| G: -5246.08711 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63944 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-1.18663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73354 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-1.28073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94432 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-1.49151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94124 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-1.48844) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70980 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-2.25699) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94225 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-1.48944) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64493 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-2.19212) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41701 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.96420) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35879 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-2.90599) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66890 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-2.21610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30257 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-2.84977) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27397 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-2.82117) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66082 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-2.20801) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58724 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-2.13443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20134 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.74853) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13127 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.67846) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32229 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.86949) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16067 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.70787) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17730 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.72449) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28601 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-1.83320) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22688 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-1.77407) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13741 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-1.68460) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15120 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-1.69840) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30650 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-1.85369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29023 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-1.83742) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48520 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-2.03239) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42632 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-0.97351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19761 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.74480) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31843 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.86562) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41696 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.96415) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28772 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-1.83492) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27151 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-1.81870) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15553 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.70273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98315 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-1.53034) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07534 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.62253) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92698 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.47418) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06247 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-1.60966) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13425 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-1.68145) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80573 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-1.35292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76222 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-1.30941) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92274 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-1.46993) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.33260 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (2.12020) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.73971 HOMO: -7.36340 LUMO: -1.04492 factor:1 | -1 (1.71309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.64194 HOMO: -6.65863 LUMO: -0.41906 factor:1 | -1 (1.81086) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.86181 HOMO: -7.15115 LUMO: -0.66396 factor:1 | -1 (1.59100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.80399 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (1.64882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.99422 HOMO: -7.20285 LUMO: 0.47892 factor:1 | -1 (1.45858) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88810 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-1.43529) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83381 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.38101) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67144 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-1.21863) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42227 HOMO: -6.70761 LUMO: 1.95650 factor:1 | -1 (0.03053) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22222 HOMO: -6.60420 LUMO: 1.80684 factor:1 | -1 (0.23059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47909 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.02629) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59890 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.14610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90891 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.45611) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44148 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.98867) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21630 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.76350) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43380 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.98100) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96918 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-2.51637) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69246 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-3.23965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00796 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-2.55515) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00858 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-2.55578) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03049 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-1.57769) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04018 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.58738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56072 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.10791) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57865 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.12584) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81022 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.35741) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69751 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.24470) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74548 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.29268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74519 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.29239) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73844 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.28564) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02093 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.56812) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66269 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.20988) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73060 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-1.27779) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68608 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-1.23327) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81038 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-1.35758) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10647 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.65366) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06660 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.61380) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50253 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-2.04972) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29145 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.83865) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69199 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-3.23919) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94945 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-2.49664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88542 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-2.43262) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05103 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-2.59822) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37241 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.91960) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31907 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-1.86627) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64515 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-2.19234) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62427 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-2.17147) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72898 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-2.27618) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49418 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-2.04137) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82135 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-1.36854) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59128 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.13847) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70456 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.25175) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27442 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.82161) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30038 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.84757) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34892 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.89612) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41896 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.96616) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46185 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-2.00904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08145 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-2.62865) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55899 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-2.10619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57339 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-2.12058) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82935 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-1.37654) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30618 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.85338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06991 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.61710) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23943 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.78663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45699 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-1.00418) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12783 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-1.67502) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87408 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-1.42128) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14274 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.68994) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28950 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.83670) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20879 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.75599) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38118 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.92837) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27489 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.82208) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06426 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.61146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93106 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-2.47825) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58974 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-2.13694) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33284 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.88003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58006 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-2.12725) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54080 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.08799) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30346 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.85066) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22969 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.77689) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25663 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-0.80382) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53703 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-0.08422) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60666 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-0.15385) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49866 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-0.04585) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90478 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.45197) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13104 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.67824) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03860 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.58580) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09429 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-0.64148) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97992 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-0.52711) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12291 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.67011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17334 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.72053) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14746 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.69465) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95717 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.50436) | 1 | 1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09821 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.64540) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18977 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.73697) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07233 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.61952) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85270 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-0.39990) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09002 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.63721) | -1 | -1 |
| G: -5246.08711 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23383 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.78102) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72370 HOMO: -6.58243 LUMO: 0.28028 factor:1 | -1 (0.72910) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06676 HOMO: -6.79468 LUMO: 0.14966 factor:1 | -1 (0.38605) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06589 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.38692) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37568 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-0.92287) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38534 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-0.93253) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33481 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-0.88200) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42983 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-0.97702) | 1 | 1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73961 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.28680) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48268 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.02987) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61705 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.16424) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39813 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.94532) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50325 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.05044) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06675 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.61394) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38412 HOMO: -6.48992 LUMO: 1.08301 factor:1 | -1 (0.06868) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41468 HOMO: -7.18381 LUMO: 1.61908 factor:1 | -1 (0.03812) | 1 | 1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36007 HOMO: -6.74842 LUMO: 0.57960 factor:1 | -1 (0.09274) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47436 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.02155) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37904 HOMO: -6.74570 LUMO: 0.77280 factor:1 | -1 (0.07377) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48712 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-0.03431) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98576 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.53295) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93648 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.48367) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66360 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-2.21079) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16399 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-2.71118) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37064 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.91783) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64139 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-2.18858) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52275 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-2.06994) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28561 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.83280) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47897 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-1.02617) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38833 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.93553) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54627 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-1.09346) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54053 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-1.08772) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61214 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-2.15933) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55946 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-2.10665) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69067 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-2.23786) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85612 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.40331) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98592 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.53312) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15017 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.69736) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18065 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.72784) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09112 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.63832) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15532 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.70252) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23058 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.77777) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43769 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.98488) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48079 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-2.02798) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49722 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-2.04442) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57568 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.12288) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65408 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-1.20127) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67111 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-1.21831) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79294 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-1.34013) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04331 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.59051) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86744 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.41464) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85085 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.39804) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24663 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.79383) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15235 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.69954) | -1 | -1 |
| G: -5246.08711 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69125 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-1.23844) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99964 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.54683) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24971 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.79690) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14486 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.69206) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23491 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.78210) | 1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35331 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.90051) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45740 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.00459) | -1 | -1 |
| G: -5246.08711 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51408 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.06127) | 1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26456 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-2.81175) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.79654 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-3.34374) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88970 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.43690) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73239 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.27958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95523 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.50242) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01655 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-2.56375) | -1 | -1 |
| G: -5246.08711 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02148 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-2.56867) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67348 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-1.22068) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79010 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-2.33729) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87712 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-2.42432) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67666 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-2.22385) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09404 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.64124) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29402 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.84121) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46123 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.00843) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07711 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.62430) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10133 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.64852) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05740 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-2.60459) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06771 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-2.61491) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83263 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-2.37983) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03432 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-2.58152) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81449 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-1.36168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56882 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-2.11601) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63334 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-2.18053) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55987 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-2.10706) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63687 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-2.18407) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71373 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-1.26092) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51805 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-1.06524) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90940 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-2.45659) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49900 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.04620) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11683 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-2.66402) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50830 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-2.05549) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00301 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.55021) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78853 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.33573) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84905 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-1.39624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00337 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-1.55056) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89202 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-1.43921) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60017 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.14737) | -1 | -1 |
| G: -5246.08711 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49653 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.04372) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82197 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.36917) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70782 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.25502) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21869 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.76588) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10613 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.65333) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71951 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.26671) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78671 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.33390) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64517 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.19237) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60973 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.15692) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90929 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.45648) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64686 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.19405) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39879 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.94599) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.76487) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65964 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-3.20683) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05405 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.60125) | 1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39336 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.94055) | 1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19150 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.73869) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46035 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.00755) | 1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67647 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.22366) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27958 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.82677) | 1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56904 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.11623) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87462 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.42181) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50503 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.05223) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54738 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.09457) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22505 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.77224) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.63341 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-3.18060) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01955 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.56674) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72996 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.27716) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24886 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.79605) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82044 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.36764) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76223 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-3.30942) | -1 | -1 |
| G: -5246.08711 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21109 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.75828) | 1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44846 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.99566) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67249 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.21969) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01049 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.55768) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93076 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.47795) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58572 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.13292) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69427 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.24147) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07992 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.62711) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11995 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.66714) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19489 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.74208) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32441 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.87161) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21121 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.75841) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24539 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.79259) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46676 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.01395) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42501 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.97221) | 1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29233 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.83953) | 1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09435 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.64155) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90934 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.45654) | 1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26282 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.81001) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10091 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.64810) | 1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25979 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.80698) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36126 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.90845) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96746 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.51466) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89008 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.43727) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85878 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.40598) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01157 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.55877) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42151 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.96871) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38778 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.93497) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51769 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.06488) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56836 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.11555) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39576 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.94296) | -1 | -1 |
| G: -5246.08711 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37908 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.92628) | 1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18229 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.72948) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04596 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.59315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06852 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.61571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40477 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.95196) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15198 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.69917) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58417 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.13136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69472 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.24192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60821 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.15540) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71755 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.26474) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86827 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.41546) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35997 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.90716) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50648 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.94633) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45170 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.00111) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52985 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.92296) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94292 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.50989) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99334 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.45946) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04610 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.40670) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17250 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.28030) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28241 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.17040) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83026 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.37746) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90181 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.44901) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82807 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.37526) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92007 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.46727) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58747 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.13466) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48776 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.03496) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48123 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.02843) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63514 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.18233) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43068 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.02212) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36263 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.09018) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34407 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.10874) | -1 | -1 |
| G: -5246.08711 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36992 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.08289) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48851 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.03570) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49945 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.04664) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72660 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.27379) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59611 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.14330) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85041 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.39760) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82045 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.36764) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84815 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.39535) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95907 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.50626) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70271 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.24990) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81718 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.36438) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77264 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.31983) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42150 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.96869) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20660 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.24621) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32595 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.12686) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49093 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.03812) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45540 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.00259) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07439 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.62158) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37684 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.92404) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40079 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.94798) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46977 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.01696) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48882 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.03601) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48155 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.02874) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68670 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.23389) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64826 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.19545) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83879 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.38598) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58170 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.12889) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65916 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.79365) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99925 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.45356) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72542 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.72739) | -1 | -1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25294 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.19987) | 1 | 1 |
| G: -5246.08711 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52590 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.07309) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53566 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.08286) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79151 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.33870) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58475 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.13195) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60285 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.15004) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.54597) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58160 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.12879) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05501 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.60221) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20696 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.75415) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98619 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.53339) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09477 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.64196) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91052 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.45771) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17137 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.71856) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12889 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.67609) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34222 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.88941) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37134 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.91854) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54574 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.09294) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59867 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.14586) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31872 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (1.13409) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33774 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (1.11507) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49222 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.96059) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81957 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.63324) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76198 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.30918) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85815 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.40534) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09856 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.64575) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91216 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.45936) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21528 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.23753) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20788 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.24493) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34761 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.10520) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62114 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.16833) | -1 | -1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94226 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.48945) | 1 | 1 |
| G: -5246.08711 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86185 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.40904) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06604 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.61324) | 1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86830 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-0.41549) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32193 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-1.86912) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.49270 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-3.03989) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49399 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-2.04118) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58011 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-2.12730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50931 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-2.05650) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45951 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.00670) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15578 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.70297) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34451 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.89171) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38832 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-1.93552) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20337 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.75056) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04032 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.58751) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24258 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.78977) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40218 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.94937) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10495 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.65214) | -1 | -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: -6.05181 LUMO: 0.35103 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: -11512.17409 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.72128) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97969 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.52689) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57048 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-2.11767) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25904 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.80624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49728 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-2.04447) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40598 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.95318) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25990 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-0.80709) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45922 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-1.00641) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09978 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-0.64698) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85085 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.39805) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09785 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.64505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97586 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-0.52306) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32876 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.87595) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23677 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-0.78396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49718 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.04437) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53933 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.08652) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12870 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.67589) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98889 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.53608) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14535 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.69255) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08973 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.63693) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39291 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-2.94011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00257 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.54976) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87622 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-2.42342) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02689 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-2.57409) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18616 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-2.73336) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98319 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-2.53039) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51291 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.06010) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70505 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.25224) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55480 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.10200) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77013 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-2.31732) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22487 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.77207) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56240 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.10960) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73530 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-2.28249) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36323 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-2.91042) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81527 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-2.36247) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56047 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.10767) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82116 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.36835) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49529 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-2.04249) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67619 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-2.22339) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42246 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.96965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47661 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-1.02380) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66074 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-2.20793) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84741 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-2.39460) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41735 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-2.96454) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23718 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-2.78438) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59592 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-2.14311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72009 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-2.26728) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74888 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-2.29607) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24384 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-0.79103) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21456 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-0.76176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01869 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-0.56589) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33171 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-0.87890) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17731 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.72450) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15091 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.69811) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72618 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-2.27338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85497 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-2.40217) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92858 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-2.47577) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07842 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.62562) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18961 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.73680) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15502 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.70222) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25470 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.80189) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23489 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.78208) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39960 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.94679) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19657 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.74377) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15475 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.70194) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09113 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.63832) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67064 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-2.21784) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79671 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-2.34391) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04700 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-2.59420) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59826 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-2.14545) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71375 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-2.26094) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94980 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-2.49700) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62978 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.17697) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11366 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.66086) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00963 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.55683) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21881 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.76600) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21696 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.76415) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24512 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.79231) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12199 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.66918) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79370 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.34090) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12674 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.67394) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49868 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.04587) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73313 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-1.28032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84363 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.39083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05099 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-1.59818) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49545 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.04264) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70821 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.25541) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51128 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.05848) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44428 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-0.99147) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26410 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-1.81130) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63876 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-1.18595) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63601 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.18321) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28689 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.83408) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51187 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.05907) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60522 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.15241) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71978 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.26697) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72789 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.27508) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83094 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-0.37813) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66489 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-0.21209) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45028 HOMO: -7.52123 LUMO: 0.06803 factor:1 | -1 (0.00253) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74726 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.29445) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73322 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-0.28041) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74024 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.28743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64182 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.18901) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35748 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.09532) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64342 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-0.19062) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74353 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-0.29073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86375 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-0.41095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71523 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-0.26243) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75610 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.30330) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85347 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.40066) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80340 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-0.35059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72998 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-0.27718) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65490 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.20210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36347 HOMO: -5.90759 LUMO: 2.00820 factor:1 | -1 (0.08933) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65074 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.19794) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57316 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.12036) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59665 HOMO: -6.16882 LUMO: 1.94017 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: -11510.65333 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.20052) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79295 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.34014) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32741 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.87460) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38278 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.92998) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22006 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.76725) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14806 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-0.69525) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72965 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.27684) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52280 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-2.07000) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77011 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.31730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59253 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-1.13972) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86644 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-1.41363) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67959 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-0.22678) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68568 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-0.23288) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65186 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.19905) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49262 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-0.03981) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57564 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-0.12283) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41468 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (0.03812) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89713 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.44433) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62038 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-2.16758) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54083 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-0.08803) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22766 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (0.22515) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26898 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.81617) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30006 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.84725) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53944 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.08663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02815 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-1.57535) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96200 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.50920) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44424 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.99144) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88956 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-2.43675) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53402 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-1.08122) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73054 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.27774) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15417 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-1.70136) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06402 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.61121) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11044 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-1.65764) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58150 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-2.12869) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71920 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-1.26639) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85144 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.39864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30838 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.85557) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83013 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.37732) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77398 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.32118) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62934 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-1.17654) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78691 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.33410) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56488 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-1.11207) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48727 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-1.03447) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75144 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-1.29864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32794 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-1.87514) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79242 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-1.33962) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78463 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-2.33183) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.56791 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-3.11511) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71867 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-2.26586) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57376 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.12095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45255 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.99975) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91031 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.45751) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31274 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-0.85993) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14459 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-1.69179) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59998 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.14718) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05838 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-2.60557) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78569 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-2.33289) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37241 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.91961) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27377 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.82097) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14190 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.68909) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58211 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-1.12930) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39564 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-2.94283) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82901 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-2.37621) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11879 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-2.66598) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61222 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-2.15941) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.39517 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-2.94237) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81040 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-2.35759) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73634 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.28353) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68929 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.23649) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41045 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.95764) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30498 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.85217) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88290 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-1.43009) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67992 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-2.22712) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67609 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-2.22328) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24479 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-0.79199) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43684 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-1.98404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30813 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-1.85533) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48404 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-1.03123) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67471 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-1.22190) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27524 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-0.82244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68600 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-1.23319) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20821 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-1.75541) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28811 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.83531) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51141 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-1.05860) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04942 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.59661) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50745 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.05464) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19479 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (0.25802) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21520 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (0.23761) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50473 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.05192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38973 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (0.06308) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10034 HOMO: -6.83550 LUMO: -0.77825 factor:1 | -1 (0.35247) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06635 HOMO: -7.14843 LUMO: 0.44627 factor:1 | -1 (0.38646) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36704 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (0.08577) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09277 HOMO: -6.81373 LUMO: -0.93879 factor:1 | -1 (0.36003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87007 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (0.58273) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40851 HOMO: -7.13483 LUMO: -1.25444 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: -11510.27525 HOMO: -6.37835 LUMO: -1.54289 factor:1 | -1 (0.17755) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09855 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-1.64574) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68461 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-1.23181) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73820 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-0.28539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35923 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (0.09358) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60891 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.15610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70028 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.24748) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31312 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-0.86032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32116 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (0.13165) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33705 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (0.11576) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04213 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (0.41067) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51107 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-0.05826) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57364 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.12084) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64875 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.19594) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24395 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-0.79114) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48942 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.03662) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65460 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.20179) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29119 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-0.83838) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61484 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.16204) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74644 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.29363) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37184 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.91904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40063 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.94783) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51628 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.06348) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09442 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.64162) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30899 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.85618) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80627 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.35347) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39163 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.93882) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06759 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.61479) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93365 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.48084) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94383 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-1.49102) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68861 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-1.23581) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55218 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-0.09938) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59115 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-0.13834) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23128 HOMO: -6.35658 LUMO: -0.82995 factor:1 | -1 (0.22153) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76000 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.30719) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61838 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-1.16557) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66151 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.20870) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32044 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.86764) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93262 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.47981) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16247 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.70966) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72399 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.27118) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49772 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.04492) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75079 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.29798) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37037 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.91757) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25309 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-0.80029) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35410 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-0.90130) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11989 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-0.66709) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37672 HOMO: -6.73754 LUMO: -2.58780 factor:1 | -1 (0.07608) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56326 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-0.11045) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16105 HOMO: -6.98788 LUMO: 0.34831 factor:1 | -1 (0.29176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59803 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.14523) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38619 HOMO: -6.67767 LUMO: -0.82450 factor:1 | -1 (0.06661) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43098 HOMO: -6.84911 LUMO: -0.21497 factor:1 | -1 (0.02182) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09468 HOMO: -6.23141 LUMO: 0.21769 factor:1 | -1 (0.35813) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53096 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.07815) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55166 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.09885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66603 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.21322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41100 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.95819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49024 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.03743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27534 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.82254) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58004 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-1.12723) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31347 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-0.86067) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21685 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.76404) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29443 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.84162) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07608 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.62328) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67653 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.22372) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36235 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.90954) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10504 HOMO: -7.36340 LUMO: 0.29116 factor:1 | -1 (0.34776) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31566 HOMO: -6.64230 LUMO: -0.79185 factor:1 | -1 (0.13715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73631 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.28351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43691 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-0.98410) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71852 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.26571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40345 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.95065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45786 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.00505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19097 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.73816) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94533 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.49253) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56668 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.11387) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31924 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.86644) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45582 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.00301) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26953 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.81672) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10575 HOMO: -6.65318 LUMO: -0.94696 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: -11510.26216 HOMO: -6.96067 LUMO: -1.03675 factor:1 | -1 (0.19064) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04619 HOMO: -6.23141 LUMO: -0.66396 factor:1 | -1 (0.40662) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70165 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.24884) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30468 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.85187) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43549 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.98268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03504 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-1.58223) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12177 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.66896) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31590 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.86309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08299 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-0.63019) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11815 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-0.66535) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29045 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.83765) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92086 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-1.46805) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15325 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-0.70045) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09668 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.64388) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31165 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-0.85885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48181 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.02901) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50298 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.05018) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25775 HOMO: -6.32937 LUMO: -1.89119 factor:1 | -1 (0.19505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56122 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-0.10841) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72840 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-0.27560) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68701 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-0.23421) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31539 HOMO: -6.31304 LUMO: -0.57960 factor:1 | -1 (0.13742) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89827 HOMO: -6.94435 LUMO: -0.74287 factor:1 | -1 (0.55454) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00670 HOMO: -6.35658 LUMO: -1.53472 factor:1 | -1 (0.44610) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.77304 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (0.67977) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25920 HOMO: -7.05319 LUMO: -0.33198 factor:1 | -1 (0.19361) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.13765 HOMO: -6.68040 LUMO: -0.09252 factor:1 | -1 (1.31515) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35733 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (1.09548) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.07180 HOMO: -6.59604 LUMO: -1.45853 factor:1 | -1 (1.38101) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67802 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (0.77479) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.36089 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (1.09191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49902 HOMO: -7.14027 LUMO: -0.81634 factor:1 | -1 (0.95379) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.20353 HOMO: -6.80285 LUMO: -0.74287 factor:1 | -1 (1.24927) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25123 HOMO: -6.53890 LUMO: -1.13471 factor:1 | -1 (1.20157) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64287 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-1.19006) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20375 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-1.75094) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77174 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-1.31894) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59740 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-1.14459) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86190 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.40910) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56312 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.11031) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10430 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.65150) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81866 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.36586) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36129 HOMO: -6.64774 LUMO: -0.66124 factor:1 | -1 (0.09151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64035 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.18754) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20573 HOMO: -6.52529 LUMO: -0.68301 factor:1 | -1 (0.24708) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86860 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.41579) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76586 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.31306) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48327 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-1.03047) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78840 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-1.33559) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53299 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-1.08018) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62246 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.16965) | -1 | -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: -6.35658 LUMO: -0.58232 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: -11511.63601 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-1.18321) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15154 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.69873) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63971 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-1.18691) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80863 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-2.35583) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86656 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-2.41376) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49039 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-2.03759) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00483 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-2.55202) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.77681 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-3.32401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11209 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-2.65929) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76346 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-2.31065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67866 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.22585) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72838 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.27557) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76359 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.31078) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50788 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.05508) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71208 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-0.25927) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57618 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.12338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21582 HOMO: -6.73482 LUMO: 0.62858 factor:1 | -1 (0.23698) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98827 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.53547) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99091 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.53811) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61050 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.15769) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49961 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-0.04680) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12537 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-2.67257) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13909 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.68628) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76352 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-2.31071) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37615 HOMO: -6.49808 LUMO: -0.51157 factor:1 | -1 (0.07665) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65390 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.20109) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52432 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.07151) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15707 HOMO: -6.75931 LUMO: 1.13744 factor:1 | -1 (0.29573) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74095 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.28814) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25512 HOMO: -6.59604 LUMO: 1.19458 factor:1 | -1 (0.19769) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38168 HOMO: -7.09401 LUMO: 0.60137 factor:1 | -1 (0.07113) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46173 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.00893) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12474 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.67193) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13350 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.68069) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.91983) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63858 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.18577) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13699 HOMO: -6.58788 LUMO: -1.03947 factor:1 | -1 (0.31582) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48195 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.02914) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11065 HOMO: -6.63958 LUMO: -1.52112 factor:1 | -1 (0.34216) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46647 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-0.01366) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31386 HOMO: -6.22324 LUMO: -0.87893 factor:1 | -1 (0.13894) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72628 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.27347) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68207 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-2.22927) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65466 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.20185) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36431 HOMO: -6.49536 LUMO: -0.63403 factor:1 | -1 (0.08849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59714 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.14433) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50402 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.05121) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24701 HOMO: -7.20285 LUMO: 0.10612 factor:1 | -1 (0.20580) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50677 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.05396) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67471 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.22191) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63501 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.18221) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31637 HOMO: -6.48719 LUMO: 0.16871 factor:1 | -1 (0.13644) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39086 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.93805) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44742 HOMO: -6.68856 LUMO: -0.78641 factor:1 | -1 (0.00539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40965 HOMO: -6.56883 LUMO: -1.00682 factor:1 | -1 (0.04316) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09598 HOMO: -6.41100 LUMO: -0.48980 factor:1 | -1 (0.35682) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41569 HOMO: -6.52257 LUMO: -0.59865 factor:1 | -1 (0.03712) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87845 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.42564) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96345 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.51065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58802 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.13521) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48724 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-2.03443) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19783 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.74502) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15244 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.69963) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10248 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.64967) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31084 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.85803) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25107 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.79826) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57290 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-2.12009) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13985 HOMO: -6.07630 LUMO: 1.81500 factor:1 | -1 (0.31296) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50883 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.05603) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81148 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.35867) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70323 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.25043) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47117 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-0.01837) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71685 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-2.26404) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44274 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.01007) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49430 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-0.04150) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57474 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.12193) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44725 HOMO: -6.41372 LUMO: -0.20409 factor:1 | -1 (0.00555) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27686 HOMO: -7.18381 LUMO: 0.42722 factor:1 | -1 (0.17595) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59507 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-0.14226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38756 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.93476) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23695 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.78414) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56536 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-2.11256) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12885 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.67604) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22966 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.77686) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13404 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.68124) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79341 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-0.34060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13949 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.68668) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07940 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.62660) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53668 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.91613) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76806 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.68475) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26816 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (1.18465) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31747 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (1.13534) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.55127 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (0.90154) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78527 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.33246) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31284 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.86003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89027 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-1.43747) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48466 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.03186) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.30057 HOMO: -6.26678 LUMO: 1.95922 factor:1 | -1 (1.15224) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45317 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.99964) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.16993 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (1.28288) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58155 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.87125) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70887 HOMO: -6.14161 LUMO: 1.77690 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: -11509.99443 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.45838) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31718 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (0.13562) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16850 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (0.28430) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78147 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.67133) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45237 HOMO: -6.70216 LUMO: -0.65035 factor:1 | -1 (0.00044) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25528 HOMO: -6.79468 LUMO: -0.83811 factor:1 | -1 (0.19753) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95187 HOMO: -6.99877 LUMO: -0.79729 factor:1 | -1 (0.50093) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12994 HOMO: -7.08040 LUMO: -0.85444 factor:1 | -1 (0.32286) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47477 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.02196) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06118 HOMO: -7.05047 LUMO: 0.13878 factor:1 | -1 (0.39163) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03840 HOMO: -6.90897 LUMO: -0.77552 factor:1 | -1 (0.41440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01955 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.43326) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72847 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (0.72434) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29882 HOMO: -6.78108 LUMO: -0.81634 factor:1 | -1 (0.15399) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10036 HOMO: -6.74570 LUMO: -0.77280 factor:1 | -1 (0.35244) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16472 HOMO: -7.28177 LUMO: -1.68438 factor:1 | -1 (0.28809) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11563 HOMO: -7.22190 LUMO: -1.63540 factor:1 | -1 (0.33718) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98648 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (0.46632) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92988 HOMO: -6.57971 LUMO: -0.93063 factor:1 | -1 (0.52292) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83516 HOMO: -6.88176 LUMO: 0.58232 factor:1 | -1 (0.61764) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31275 HOMO: -6.85727 LUMO: 0.51430 factor:1 | -1 (0.14006) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31528 HOMO: -6.83550 LUMO: 0.87893 factor:1 | -1 (0.13753) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45408 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.00128) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72285 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.27005) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67787 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-0.22507) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75069 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-0.29788) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69107 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-0.23826) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97592 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-0.52311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03178 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-0.57898) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99094 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.53813) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34278 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.88998) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57952 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.12671) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74415 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-1.29134) | 1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88652 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-1.43371) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42756 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-1.97476) | 1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51095 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.05814) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30855 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.85574) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14098 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.68818) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42632 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.97351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14283 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.69003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84334 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.39054) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68729 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.23448) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83330 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.38050) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67580 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.22300) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75023 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.29742) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79409 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.34129) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85010 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-2.39730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11357 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-1.66077) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03107 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-1.57826) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15540 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-1.70259) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81831 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-0.36550) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43172 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.02109) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36029 HOMO: -6.91169 LUMO: 0.88981 factor:1 | -1 (0.09252) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49398 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-0.04117) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65216 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.19935) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54767 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.90513) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65342 HOMO: -6.43821 LUMO: -1.00410 factor:1 | -1 (0.79939) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73347 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.71933) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.38509 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (1.06772) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60625 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-0.15345) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61033 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.15753) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67082 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-0.21802) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81692 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.36412) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55313 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-1.10032) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75998 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-2.30717) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15537 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.70256) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00538 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.55257) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26361 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.81081) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55653 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.10372) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04199 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-0.58918) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15342 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-0.70061) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87164 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.41884) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90427 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.45146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64652 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.19372) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77937 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-0.32656) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75161 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-0.29881) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89956 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-0.44676) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91876 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.46596) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78771 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.33491) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10209 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.64928) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86225 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-1.40944) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12647 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-1.67366) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89297 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-1.44016) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96511 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-1.51230) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50961 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-2.05680) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89757 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.44476) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65136 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-1.19855) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34252 HOMO: -6.78924 LUMO: -0.84900 factor:1 | -1 (0.11029) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55452 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.10172) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35237 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (0.10044) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40774 HOMO: -6.56339 LUMO: -0.68573 factor:1 | -1 (0.04506) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09609 HOMO: -6.31032 LUMO: -0.31837 factor:1 | -1 (0.35671) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23024 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (0.22256) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46649 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-0.01369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84728 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-1.39447) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41250 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-0.95969) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62281 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-1.17001) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91808 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-1.46528) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50977 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-2.05696) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91811 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-1.46531) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96979 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.51698) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64311 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.19031) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85308 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-1.40027) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40730 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-0.95449) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66728 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-1.21447) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47111 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-1.01830) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35184 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-0.89904) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64619 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.19338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35786 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-0.90505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55147 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.09866) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77253 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.31973) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85368 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-1.40087) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71778 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-1.26498) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51334 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-1.06054) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42008 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-1.96727) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17756 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-2.72476) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64615 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-2.19335) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32721 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-1.87440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53932 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-2.08651) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84845 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-1.39564) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81569 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-1.36288) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86260 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.40979) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76665 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.31385) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49712 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.04432) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68249 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.22968) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72004 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-1.26723) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25239 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.79958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55481 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.10201) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45427 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.00146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19720 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.74439) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10819 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.65539) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32210 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.86929) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94167 HOMO: -7.28721 LUMO: 0.23946 factor:1 | -1 (0.51114) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94738 HOMO: -6.71849 LUMO: -0.56600 factor:1 | -1 (0.50542) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84403 HOMO: -6.85183 LUMO: -0.84355 factor:1 | -1 (0.60877) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89495 HOMO: -6.53345 LUMO: -0.84627 factor:1 | -1 (0.55786) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65780 HOMO: -6.60148 LUMO: -0.63130 factor:1 | -1 (0.79501) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44811 HOMO: -6.36202 LUMO: -0.60137 factor:1 | -1 (1.00470) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68689 HOMO: -6.28855 LUMO: -0.52790 factor:1 | -1 (0.76592) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46358 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-0.01078) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20102 HOMO: -6.36202 LUMO: -0.24218 factor:1 | -1 (0.25179) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23280 HOMO: -6.43549 LUMO: 0.14150 factor:1 | -1 (0.22000) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44464 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.00816) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37417 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (0.07864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36347 HOMO: -6.33753 LUMO: -0.02993 factor:1 | -1 (0.08933) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89470 HOMO: -6.49808 LUMO: -0.83811 factor:1 | -1 (0.55811) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.27959 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (1.17322) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56893 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (0.88388) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24702 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-0.79422) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98392 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-0.53111) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90569 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-0.45288) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21682 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-0.76401) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30640 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.85359) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91514 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.53767) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.94191 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (0.51089) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89353 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.55928) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81938 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.63343) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.43439 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (1.01841) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58686 HOMO: -6.34297 LUMO: -0.50341 factor:1 | -1 (0.86595) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71747 HOMO: -6.20692 LUMO: -0.51974 factor:1 | -1 (0.73533) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45653 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-0.00373) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02823 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (0.42458) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30513 HOMO: -6.41917 LUMO: 0.19320 factor:1 | -1 (0.14768) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53977 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-0.08697) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16344 HOMO: -6.56339 LUMO: 0.36735 factor:1 | -1 (0.28937) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13900 HOMO: -6.54978 LUMO: 1.12655 factor:1 | -1 (0.31380) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84414 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (0.60866) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84417 HOMO: -6.29944 LUMO: 1.40955 factor:1 | -1 (0.60864) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07329 HOMO: -6.74842 LUMO: 0.74015 factor:1 | -1 (0.37952) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07457 HOMO: -6.15522 LUMO: 1.94289 factor:1 | -1 (0.37824) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17269 HOMO: -6.20147 LUMO: 1.40139 factor:1 | -1 (0.28011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83104 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.37823) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67354 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.22073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73775 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.28495) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34401 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.89120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57087 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.11806) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49604 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.04323) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88105 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-1.42824) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75894 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-2.30614) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22472 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-2.77192) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10502 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-2.65221) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28936 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.83655) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52776 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.07495) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87577 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.42297) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24202 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.78921) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94345 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-0.49065) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51153 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-0.05872) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22958 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-0.77678) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75855 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-0.30575) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36322 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.91041) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46298 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-0.01018) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17566 HOMO: -6.60420 LUMO: 1.40955 factor:1 | -1 (0.27715) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84439 HOMO: -6.81645 LUMO: 1.59731 factor:1 | -1 (0.60842) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47071 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.01791) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09840 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.35440) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29422 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.15859) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11083 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.65803) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46292 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.01011) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11238 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.65958) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36621 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-0.91340) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84761 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.39480) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94184 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.48903) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20415 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-2.75134) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32370 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-1.87089) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69260 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-2.23980) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28187 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.82907) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65725 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-2.20445) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11826 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.66545) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35625 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.90345) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77672 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-1.32392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.46588 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.98693) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68811 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (0.76469) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.57118 HOMO: -6.51168 LUMO: 1.92112 factor:1 | -1 (0.88162) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39613 HOMO: -6.71305 LUMO: 1.91024 factor:1 | -1 (1.05667) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32430 HOMO: -6.86815 LUMO: 2.02997 factor:1 | -1 (1.12851) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64542 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.80739) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78107 HOMO: -6.45182 LUMO: 1.66806 factor:1 | -1 (0.67174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18880 HOMO: -6.44638 LUMO: 2.16058 factor:1 | -1 (0.26400) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32796 HOMO: -6.65591 LUMO: 1.95106 factor:1 | -1 (0.12485) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96012 HOMO: -6.35114 LUMO: 1.42316 factor:1 | -1 (0.49269) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17160 HOMO: -6.48719 LUMO: 1.59187 factor:1 | -1 (0.28120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38470 HOMO: -7.05591 LUMO: 1.61908 factor:1 | -1 (0.06811) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22216 HOMO: -6.92258 LUMO: 1.87214 factor:1 | -1 (0.23064) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19212 HOMO: -5.85861 LUMO: 2.11705 factor:1 | -1 (0.26069) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10221 HOMO: -6.27767 LUMO: 1.75513 factor:1 | -1 (0.35059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21966 HOMO: -6.16882 LUMO: 1.73881 factor:1 | -1 (0.23315) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98405 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-1.53124) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78282 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.33001) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92067 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.46786) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14888 HOMO: -6.99333 LUMO: 2.08439 factor:1 | -1 (0.30392) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44723 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.00558) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24712 HOMO: -7.19741 LUMO: 2.24766 factor:1 | -1 (0.20569) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46108 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.00827) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79042 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.33761) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69964 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-0.24683) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13331 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-0.68050) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89910 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.44629) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06025 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.60744) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74563 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-0.29282) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47376 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.02095) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62514 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-0.17233) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74683 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.29402) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77706 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.32425) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42345 HOMO: -6.66135 LUMO: -0.75648 factor:1 | -1 (1.02935) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56528 HOMO: -7.56749 LUMO: 0.22585 factor:1 | -1 (0.88753) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66844 HOMO: -6.45182 LUMO: -0.71294 factor:1 | -1 (0.78437) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79941 HOMO: -6.31032 LUMO: -0.34286 factor:1 | -1 (0.65340) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07710 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.37571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12540 HOMO: -6.61781 LUMO: 1.98915 factor:1 | -1 (0.32741) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06074 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (0.39206) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28309 HOMO: -6.44094 LUMO: 1.80956 factor:1 | -1 (0.16972) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20965 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.24316) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32538 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.12743) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21316 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.23965) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16461 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.28820) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28597 HOMO: -6.74842 LUMO: -0.56872 factor:1 | -1 (0.16683) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59521 HOMO: -6.59060 LUMO: -0.22041 factor:1 | -1 (0.85759) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54185 HOMO: -6.22052 LUMO: -0.60137 factor:1 | -1 (0.91096) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70166 HOMO: -6.65863 LUMO: 0.07891 factor:1 | -1 (0.75114) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39744 HOMO: -6.57427 LUMO: 1.71160 factor:1 | -1 (1.05537) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76183 HOMO: -5.84773 LUMO: 1.99459 factor:1 | -1 (0.69098) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44073 HOMO: -6.02188 LUMO: 1.91296 factor:1 | -1 (1.01207) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80055 HOMO: -6.17698 LUMO: 2.00004 factor:1 | -1 (0.65226) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38595 HOMO: -6.02732 LUMO: 1.90752 factor:1 | -1 (0.06686) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54478 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-0.09197) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65284 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.20003) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46429 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.01148) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34766 HOMO: -6.56339 LUMO: 0.23130 factor:1 | -1 (0.10514) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58650 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-0.13369) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43321 HOMO: -6.70489 LUMO: -0.53334 factor:1 | -1 (0.01959) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20018 HOMO: -7.28993 LUMO: 0.10885 factor:1 | -1 (0.25263) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16774 HOMO: -6.22052 LUMO: 0.51974 factor:1 | -1 (0.28507) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23188 HOMO: -6.81645 LUMO: 0.25307 factor:1 | -1 (0.22093) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06929 HOMO: -6.80285 LUMO: 0.02721 factor:1 | -1 (0.38352) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93535 HOMO: -6.51441 LUMO: 0.08163 factor:1 | -1 (0.51745) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37340 HOMO: -6.73482 LUMO: -0.77008 factor:1 | -1 (0.07940) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21234 HOMO: -6.29127 LUMO: -0.44355 factor:1 | -1 (0.24047) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06921 HOMO: -6.72938 LUMO: -0.64763 factor:1 | -1 (0.38360) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07160 HOMO: -6.49264 LUMO: -0.74559 factor:1 | -1 (0.38120) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19032 HOMO: -6.67223 LUMO: -0.55239 factor:1 | -1 (0.26248) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97231 HOMO: -6.33481 LUMO: 0.33198 factor:1 | -1 (0.48050) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.85829 HOMO: -6.76475 LUMO: -0.25307 factor:1 | -1 (0.59451) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28461 HOMO: -6.65318 LUMO: 0.03810 factor:1 | -1 (0.16819) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79838 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-1.34558) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93852 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.48571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49340 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.04059) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79906 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.34626) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94413 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.49132) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79104 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-0.33824) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47517 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-0.02237) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45939 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-0.00659) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65708 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-0.20428) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60364 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-0.15083) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77986 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-0.32705) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86196 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-0.40915) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76878 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.31598) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83864 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.38583) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97423 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.52142) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02166 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.56885) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08120 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.62839) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36243 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-0.90962) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62064 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.16783) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90489 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.45208) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99093 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.53812) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71223 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-1.25942) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87455 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-1.42174) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43802 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-0.98522) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84554 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.39273) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94619 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.49339) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68186 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-1.22906) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09810 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-0.64529) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01320 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.56039) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81006 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.35725) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72341 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-2.27060) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54951 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.09670) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57819 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.12538) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70701 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.25420) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97416 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (0.47865) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14105 HOMO: -6.39468 LUMO: -0.47076 factor:1 | -1 (0.31176) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92229 HOMO: -6.31304 LUMO: 1.39594 factor:1 | -1 (0.53051) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.82681 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.62600) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11310 HOMO: -6.68312 LUMO: 1.69255 factor:1 | -1 (0.33971) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00678 HOMO: -6.61509 LUMO: 1.73881 factor:1 | -1 (0.44602) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10134 HOMO: -6.17971 LUMO: 1.90208 factor:1 | -1 (0.35146) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14242 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-0.68962) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26722 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.81441) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12223 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.66943) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31198 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-0.85917) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36945 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-0.91664) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75678 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.30397) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56591 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.11311) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62934 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-2.17653) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72121 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-1.26840) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72769 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.27488) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52915 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.07635) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79049 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.33768) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41448 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.96168) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60619 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.15338) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73808 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.28528) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21688 HOMO: -6.40828 LUMO: 1.86942 factor:1 | -1 (0.23592) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33689 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.11592) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06586 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.38695) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38336 HOMO: -6.63414 LUMO: 1.62452 factor:1 | -1 (0.06944) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29825 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.15456) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52549 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.07268) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66944 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.21663) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78786 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-0.33505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63806 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.18526) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68500 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.23219) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88881 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-0.43601) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96487 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-0.51206) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03320 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-0.58039) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30777 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-2.85496) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.99510 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-3.54230) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69393 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-0.24112) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74127 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.28846) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01990 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-2.56709) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68823 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.23542) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35632 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-2.90351) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.00011 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-3.54730) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69807 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-2.24527) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78564 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-2.33283) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00917 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-0.55636) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94400 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.49119) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16714 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-2.71434) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26848 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-2.81567) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12143 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-2.66862) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23071 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-2.77790) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.89584 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-3.44303) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88278 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-2.42998) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61567 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-3.16286) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10344 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-2.65063) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93495 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-2.48214) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98140 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-2.52859) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57019 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-1.11738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67901 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.22620) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60094 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-1.14813) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16516 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-2.71235) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.93097 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-3.47816) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23435 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-2.78155) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44019 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.98738) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55908 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-2.10627) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76751 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.31470) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88400 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.43119) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82706 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.37426) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64570 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.19289) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51672 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.06391) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78132 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.32851) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61609 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.16329) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46001 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.00720) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75036 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.29756) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88291 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.43010) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59300 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.14019) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87962 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.42681) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80876 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.35595) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78440 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.33159) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66491 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.21210) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58733 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.13452) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70731 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-1.25450) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63250 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.17970) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37511 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.92230) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83351 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.38071) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90130 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.44849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87958 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.42677) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74333 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-1.29053) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84293 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-1.39012) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75259 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-1.29978) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66505 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-1.21224) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61767 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.16487) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79294 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.34013) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91065 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-2.45784) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00336 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-2.55055) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46402 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-3.01121) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92550 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-2.47270) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17536 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-2.72255) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25607 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-2.80326) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54906 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-2.09626) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79863 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.34582) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66652 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.21371) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67634 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.22353) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62164 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.16884) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78785 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.33505) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69354 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.24073) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41734 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-0.96453) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83294 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.38013) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63106 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.17825) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64499 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.19219) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50590 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-3.05309) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92518 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-2.47237) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76434 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.31153) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49718 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.04437) | 1 | 1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40852 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.95571) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55230 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-2.09949) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68690 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.23409) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41620 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-0.96339) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.58481 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-3.13200) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86088 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-2.40807) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11811 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-2.66530) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63696 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.18416) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80129 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-1.34849) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77854 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-1.32574) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72905 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-1.27624) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60270 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-1.14990) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74946 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-1.29665) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52890 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-2.07609) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41900 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.96619) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70608 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.25327) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07234 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-2.61953) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71252 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-2.25972) | -1 | -1 |
| G: -5246.08711 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.71850 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-3.26569) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64056 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-0.18776) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40236 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (0.05045) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51360 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-0.06079) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53354 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-0.08074) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56973 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-0.11693) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25552 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.19728) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30597 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (0.14683) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86174 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-0.40893) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51297 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.06016) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08213 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (0.37067) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35381 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (0.09900) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03011 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-2.57730) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93680 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-2.48399) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68460 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-2.23180) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48609 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.03328) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30793 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (0.14487) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37904 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (0.07377) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58554 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.13274) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30691 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-1.85410) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21326 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (0.23954) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80792 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (0.64488) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44690 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.00590) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75946 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-2.30665) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76875 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-1.31594) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81988 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.36707) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42726 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-1.97446) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65843 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.20563) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60383 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-0.15102) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84530 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-0.39250) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61763 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-0.16482) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73811 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-1.28530) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74224 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.28944) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45824 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.00543) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59060 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.13779) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67558 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.22277) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54738 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.09458) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16812 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.28469) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38570 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (0.06710) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69524 HOMO: -4.45450 LUMO: 1.82044 factor:1 | -1 (0.75756) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97272 HOMO: -4.64226 LUMO: 1.70615 factor:1 | -1 (0.48009) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.47358 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.97923) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53121 HOMO: -4.85723 LUMO: 0.93607 factor:1 | -1 (0.92160) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07887 HOMO: -4.72934 LUMO: 1.00410 factor:1 | -1 (0.37394) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03310 HOMO: -4.56335 LUMO: 1.56738 factor:1 | -1 (0.41971) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87307 HOMO: -5.48854 LUMO: 0.33198 factor:1 | -1 (0.57974) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21237 HOMO: -4.97424 LUMO: 1.33608 factor:1 | -1 (0.24044) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14755 HOMO: -4.60145 LUMO: 1.74697 factor:1 | -1 (0.30526) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13193 HOMO: -5.60010 LUMO: 0.74831 factor:1 | -1 (0.32088) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16363 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.28918) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33683 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.11597) | -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: -11510.00439 HOMO: -5.79603 LUMO: 0.22313 factor:1 | -1 (0.44842) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37128 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.08153) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98091 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (0.47190) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01707 HOMO: -4.62321 LUMO: 1.82861 factor:1 | -1 (0.43574) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11971 HOMO: -5.83684 LUMO: 0.82178 factor:1 | -1 (0.33309) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92297 HOMO: -5.27629 LUMO: 0.57960 factor:1 | -1 (0.52983) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10371 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (0.34909) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72355 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-1.27074) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51685 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-1.06405) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64801 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-1.19521) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.37167 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (1.08114) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60490 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (0.84791) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.30585 HOMO: -4.44362 LUMO: 1.99187 factor:1 | -1 (1.14696) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68213 HOMO: -5.82052 LUMO: 0.43810 factor:1 | -1 (0.77068) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32721 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (1.12560) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42147 HOMO: -5.09669 LUMO: 0.72382 factor:1 | -1 (1.03134) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63252 HOMO: -6.75387 LUMO: -2.02453 factor:1 | -1 (0.82029) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23591 HOMO: -5.02322 LUMO: 1.14832 factor:1 | -1 (1.21689) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76594 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.68687) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68789 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.76491) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29493 HOMO: -5.80147 LUMO: 0.72382 factor:1 | -1 (0.15788) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19337 HOMO: -6.16066 LUMO: 0.39457 factor:1 | -1 (0.25943) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38682 HOMO: -5.98650 LUMO: 0.76736 factor:1 | -1 (0.06599) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54014 HOMO: -4.74839 LUMO: 1.88847 factor:1 | -1 (0.91267) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54416 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (0.90864) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33483 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (1.11798) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.28756 HOMO: -5.09397 LUMO: 0.98505 factor:1 | -1 (1.16525) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32960 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (1.12320) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89426 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.44145) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77515 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.32235) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90125 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.44844) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85088 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.39808) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36535 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (0.08746) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43408 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.01872) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35247 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.89966) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38771 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-0.93490) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59022 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-0.13742) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66625 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-0.21345) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37111 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-0.91830) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56782 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.11501) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73354 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.28073) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75473 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-1.30193) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31461 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.86180) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62823 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-1.17542) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03838 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-2.58557) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24283 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.79002) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35902 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-1.90621) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89969 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-1.44688) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82940 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-1.37660) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11681 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-1.66400) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94109 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.48828) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01853 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.56572) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22923 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.77642) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03543 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.58262) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19685 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-0.74404) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86111 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.40831) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97956 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-0.52676) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58541 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-0.13260) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71817 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-0.26537) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51945 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.06664) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78244 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-0.32964) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39003 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (0.06278) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58059 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-0.12778) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73314 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.28033) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90538 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-1.45257) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56161 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-2.10880) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89027 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-1.43747) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98426 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.53146) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60739 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.15459) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46244 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.00963) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24260 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (0.21021) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19013 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.26267) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91035 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.54246) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29465 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (0.15815) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19612 HOMO: -7.64640 LUMO: -2.45175 factor:1 | -1 (0.25669) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23580 HOMO: -7.46953 LUMO: -1.29798 factor:1 | -1 (1.21700) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45306 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.99975) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.92529 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (1.52751) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50726 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.94554) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.14592 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (1.30688) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27514 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (0.17766) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42619 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (0.02661) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41833 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (0.03448) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23647 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.78366) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28670 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.83389) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81193 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-1.35913) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82687 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-1.37407) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76018 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.30737) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61528 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.16247) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25846 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.19434) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18592 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (0.26689) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98714 HOMO: -7.03142 LUMO: -1.12655 factor:1 | -1 (0.46567) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27269 HOMO: -7.39878 LUMO: 0.15783 factor:1 | -1 (0.18011) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18962 HOMO: -7.25728 LUMO: 0.42178 factor:1 | -1 (0.26319) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20430 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.75150) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07660 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.62379) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18017 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.72736) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05154 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.59873) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82435 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.37154) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10378 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.65098) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62722 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.17442) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35078 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.89798) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00020 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-2.54739) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55448 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-2.10167) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14350 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.69070) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52465 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-2.07185) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11960 HOMO: -7.49946 LUMO: -0.14694 factor:1 | -1 (0.33320) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76485 HOMO: -7.44231 LUMO: 0.58232 factor:1 | -1 (0.68796) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35713 HOMO: -7.36340 LUMO: -0.68301 factor:1 | -1 (0.09568) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06077 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.39203) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02869 HOMO: -7.81511 LUMO: -0.06531 factor:1 | -1 (0.42412) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02420 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.42861) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19615 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (0.25666) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90741 HOMO: -7.44776 LUMO: -1.00954 factor:1 | -1 (0.54540) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20426 HOMO: -7.47769 LUMO: -1.02859 factor:1 | -1 (0.24855) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51654 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.06373) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34478 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (0.10803) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43939 HOMO: -7.64096 LUMO: -1.43948 factor:1 | -1 (0.01342) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24703 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (0.20577) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38679 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (0.06601) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46328 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.01048) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42320 HOMO: -7.22734 LUMO: 0.31293 factor:1 | -1 (0.02961) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48483 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.03203) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57686 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.12406) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67463 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.22183) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41011 HOMO: -6.82189 LUMO: -1.15376 factor:1 | -1 (0.04269) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02003 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.56722) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54375 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.09094) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39663 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.94383) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53106 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-1.07825) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09778 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-2.64497) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23673 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.78392) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29804 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-1.84523) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36979 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.91699) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18689 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-0.73408) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26025 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-0.80744) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30904 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-0.85623) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40798 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-0.95517) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67691 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.22410) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82897 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.37616) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89095 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.43815) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52387 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-1.07107) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59985 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-1.14704) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45383 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.00103) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63947 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.18666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41084 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-0.95803) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65158 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.19877) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01361 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-0.56080) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38379 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.93098) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62774 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-1.17493) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29209 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-0.83928) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09522 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-2.64242) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71595 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-2.26314) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92382 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-2.47101) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03106 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-2.57825) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72836 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-2.27555) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81579 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-2.36298) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82648 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-2.37368) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45654 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-2.00374) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66970 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-1.21689) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31133 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.85852) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27922 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.82641) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50883 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-1.05602) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30376 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-0.85095) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45489 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-1.00209) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65672 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.20391) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33323 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.88042) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31622 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.86342) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61484 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-1.16204) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05116 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.59835) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31598 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.86317) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18047 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-0.72766) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27532 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.82252) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53016 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-1.07735) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43669 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.98388) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34920 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-0.89640) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52001 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.06720) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22106 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.76825) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35820 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.90540) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45674 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-1.00394) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74241 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-1.28960) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.31234 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-2.85954) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54947 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-2.09666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80433 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-2.35153) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34317 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-2.89037) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23024 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-2.77744) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.96321 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-3.51040) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98836 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-2.53556) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71612 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-1.26332) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70262 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-2.24981) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67359 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-1.22078) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82042 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.36762) | -1 | -1 |
| 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: -7.53483 LUMO: -1.52384 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: -11512.45175 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.99895) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21629 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-2.76348) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30440 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.85160) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45736 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-2.00455) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21895 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-2.76615) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.94332 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-3.49051) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02515 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-2.57235) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.64372 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-3.19092) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.48952 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-3.03671) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62547 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-2.17267) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83231 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-2.37950) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48094 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-0.02814) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64146 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.18866) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43112 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (0.02169) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56312 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.11031) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65969 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-0.20689) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43025 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.02256) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56813 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.11532) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37098 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-2.91818) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97081 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-2.51801) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64467 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.19187) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46394 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.01113) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59738 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.14457) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86446 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.41165) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43992 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-1.98711) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26313 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.81032) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45113 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-1.99832) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58105 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.12825) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96710 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.51430) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79619 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.34338) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55199 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.09919) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58391 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-0.13110) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21498 HOMO: -6.85183 LUMO: -1.00410 factor:1 | -1 (0.23783) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48894 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.03614) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57399 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-2.12118) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50824 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.05543) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50892 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.05611) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14379 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.30901) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24494 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.20787) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91163 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.54118) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37060 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (0.08221) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39371 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (1.05909) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.90799 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (1.54482) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.16614 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (1.28666) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79590 HOMO: -7.49129 LUMO: 0.14150 factor:1 | -1 (0.65691) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53894 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-2.08613) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91188 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.45907) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44980 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.99700) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68992 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.23711) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40173 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.05108) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93740 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (0.51541) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70079 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.75201) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15285 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (0.29995) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13013 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.32267) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44960 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (0.00321) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72567 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-1.27287) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56680 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-2.11400) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69803 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.24522) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90527 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.45246) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61460 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.16179) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84331 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-1.39050) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10588 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.65307) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46874 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-1.01594) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78597 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-1.33317) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51238 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-2.05958) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45207 HOMO: -7.58653 LUMO: -1.61091 factor:1 | -1 (0.00073) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41759 HOMO: -7.36068 LUMO: -1.14560 factor:1 | -1 (0.03521) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12175 HOMO: -6.96339 LUMO: 0.26939 factor:1 | -1 (0.33105) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26298 HOMO: -6.53617 LUMO: 0.22313 factor:1 | -1 (0.18983) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75861 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-0.30580) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71715 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (0.73566) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09530 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (0.35750) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44685 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.00596) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46077 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.00796) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31824 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.86543) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37489 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-0.92209) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45487 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-1.00206) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73522 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-1.28242) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81667 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.36386) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55843 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.10563) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88886 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.43605) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41846 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.96565) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57476 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.12195) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62249 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.16968) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59650 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-1.14369) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.94288 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (2.50992) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.22708 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (2.22573) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.92860 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (2.52421) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66103 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.20822) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94043 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.48763) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11736 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.66456) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11363 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.66083) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15211 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.69931) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53584 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-2.08303) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61226 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.15945) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54896 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.09616) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60251 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.14971) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72919 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.27639) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59314 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.14033) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95287 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.50006) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83357 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.38077) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95505 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-0.50224) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23552 HOMO: -6.38379 LUMO: 0.58232 factor:1 | -1 (0.21728) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02654 HOMO: -7.42871 LUMO: 0.40273 factor:1 | -1 (0.42627) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64897 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.19617) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17696 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (0.27584) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64933 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.19652) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01680 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (0.43601) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.80828 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (0.64453) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99402 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.45878) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00287 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.44994) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64866 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.19586) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53173 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-2.07892) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77642 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-1.32362) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49457 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-1.04176) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63435 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-1.18155) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32493 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.87212) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36768 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.91487) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35018 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-0.89738) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44523 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-0.99243) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83999 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.38718) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82551 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.37271) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82584 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.37303) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98279 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.52999) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81201 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-1.35921) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53862 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.08582) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75931 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.30650) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67443 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.22163) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75803 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-1.30522) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42351 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.97070) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33613 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.88333) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22609 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.77328) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51810 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-2.06529) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33903 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.88622) | 1 | 1 |
| 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: -5.94025 LUMO: -0.17687 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: -11511.56270 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.10990) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48717 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.03436) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60886 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.15606) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08035 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.62755) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83804 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-0.38523) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03576 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-0.58295) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72766 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.27485) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65844 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-0.20564) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09385 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-0.64105) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83605 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-0.38325) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11505 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-0.66224) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78957 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.33677) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95491 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.50210) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03891 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.58611) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34295 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-2.89015) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94325 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-2.49044) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56158 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-2.10877) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74044 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-2.28763) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51131 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.05850) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81760 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.36480) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.59349 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-3.14068) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82422 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-2.37142) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99566 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-2.54285) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41203 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-0.95923) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57125 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.11844) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22310 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.77029) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35826 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.90545) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45876 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-1.00595) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68031 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-1.22751) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61282 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-2.16001) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95348 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.50067) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34796 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-2.89516) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42385 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-2.97105) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84534 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-2.39253) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75903 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-2.30622) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98698 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-2.53417) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15959 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.70679) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27247 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.81966) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23886 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.78606) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20860 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.75580) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82974 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.37693) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19268 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.73988) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17238 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.71958) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00599 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.55318) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69742 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-2.24461) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52408 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-2.07128) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74185 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-2.28905) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45253 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.00027) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40832 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (0.04449) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59164 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.13883) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37985 HOMO: -7.52667 LUMO: -0.74287 factor:1 | -1 (0.07295) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29835 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (0.15445) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52094 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-0.06814) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82087 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-0.36806) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65507 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-0.20226) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44440 HOMO: -6.78380 LUMO: -0.88981 factor:1 | -1 (0.00841) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21316 HOMO: -6.85999 LUMO: 0.07891 factor:1 | -1 (0.23965) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31046 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (0.14234) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39501 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (0.05780) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69745 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-2.24464) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53812 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-2.08532) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74545 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-2.29264) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85878 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-2.40598) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74977 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-2.29697) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12069 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-2.66789) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81079 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-1.35798) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89425 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-1.44144) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13606 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.68325) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77004 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.31723) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77349 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.32069) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18052 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.72771) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98541 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-0.53261) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96563 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-0.51283) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13197 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-0.67917) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92421 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-1.47140) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53707 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.08426) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75743 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.30462) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44150 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.98869) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62004 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.16723) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67694 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.22413) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23962 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-0.78682) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71327 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.26047) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35305 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.09976) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35906 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.09374) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70334 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.25054) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78111 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.32831) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40750 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (0.04531) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38268 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.07012) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73393 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.28112) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20902 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (0.24379) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17296 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.27984) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59455 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.14174) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55673 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.10392) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95599 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.50318) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57604 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.12323) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21667 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.23614) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57482 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.12202) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13357 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-1.68077) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23045 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.77765) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60866 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-1.15586) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91555 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.46275) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54493 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.09213) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73365 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.28084) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55679 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-2.10398) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59528 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.14247) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71756 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.26476) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33249 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.87968) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23287 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.78007) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96649 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.51369) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68482 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-2.23201) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52785 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.07504) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28849 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.83568) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46395 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-2.01114) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31783 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.86502) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68322 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.23042) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59441 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-1.14160) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37965 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.92685) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37701 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.92421) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12861 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (0.32420) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97816 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (0.47465) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23106 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (0.22175) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21813 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-0.76532) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35345 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.90064) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11421 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-0.66140) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02844 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.57563) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49048 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.03768) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56815 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.11534) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38281 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.93000) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35149 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.89868) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43402 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.98122) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69394 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-1.24114) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42738 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.97458) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28673 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.83392) | -1 | -1 |
| 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: -6.78380 LUMO: -1.27894 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: -11511.46700 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.01420) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41114 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-0.95833) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22887 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.77607) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01755 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-0.56475) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25813 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.80532) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89316 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-1.44035) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20126 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.74845) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02169 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.56888) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24732 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.79452) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54249 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.08969) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31509 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (0.13772) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38562 HOMO: -6.74842 LUMO: -0.99594 factor:1 | -1 (0.06718) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52258 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.06977) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18456 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.26825) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36619 HOMO: -6.51713 LUMO: -0.05987 factor:1 | -1 (0.08661) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74636 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-0.29356) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43876 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.01404) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52524 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.07244) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37542 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.07739) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27781 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.17500) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21454 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (0.23826) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41566 HOMO: -7.36612 LUMO: -0.12245 factor:1 | -1 (0.03714) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21615 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (0.23666) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11196 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (0.34085) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03832 HOMO: -6.87087 LUMO: -0.08436 factor:1 | -1 (0.41448) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39093 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.06188) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23941 HOMO: -6.96339 LUMO: 0.65307 factor:1 | -1 (0.21339) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81075 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (0.64205) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67497 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.77784) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92752 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.52529) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80585 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.35304) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09423 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.64143) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84196 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.38915) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08052 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.62771) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27754 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.17527) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54454 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.09173) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65590 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.20310) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33763 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-1.88482) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61813 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-1.16533) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49059 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-1.03779) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71925 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-1.26645) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54789 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.90491) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.50756 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (0.94524) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.41333 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (1.03947) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.47124 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.98157) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60993 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.84287) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70517 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (0.74763) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35712 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.90432) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60461 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.15180) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22239 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.76958) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69348 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-1.24068) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61819 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.16538) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51517 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.06236) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76105 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.30824) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35984 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-0.90704) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61223 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.15942) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75728 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.69552) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01364 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (0.43916) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.04576 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (1.40705) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25670 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (1.19610) | 1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.01985 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (1.43295) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05395 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (1.39886) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24375 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (1.20906) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.36125 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (1.09156) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79875 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.65405) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67391 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.77890) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72743 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (0.72537) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88909 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.56371) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01829 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (0.43451) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.75534 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-3.30254) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91587 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-2.46307) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15220 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-2.69940) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25503 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (0.19777) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50375 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.05094) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34447 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.89166) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57119 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.11839) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68926 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-2.23645) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91176 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-2.45896) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33269 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.87988) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56270 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.10990) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.77213 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-3.31933) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93225 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-2.47945) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18037 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-2.72756) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32146 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.13135) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23781 HOMO: -6.90897 LUMO: -0.81090 factor:1 | -1 (0.21500) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54998 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.09717) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86931 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.58349) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64101 HOMO: -6.93074 LUMO: -1.25444 factor:1 | -1 (0.81180) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84420 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.60861) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.12818 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (1.32462) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.88116 HOMO: -7.39061 LUMO: -0.19320 factor:1 | -1 (1.57165) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.07923 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (1.37358) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26647 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (1.18633) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.17373 HOMO: -6.75931 LUMO: -0.73199 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: -11509.34949 HOMO: -5.45044 LUMO: -0.18776 factor:1 | -1 (1.10331) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13975 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-1.68694) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63190 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.17910) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35078 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-0.89798) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58156 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.12876) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51482 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-0.06201) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89192 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-0.43911) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60171 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-0.14890) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82046 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.36765) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42959 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.02321) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16486 HOMO: -6.60420 LUMO: -0.45715 factor:1 | -1 (0.28795) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35297 HOMO: -6.59060 LUMO: -0.58232 factor:1 | -1 (0.09984) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44967 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.99686) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57694 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.12413) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39582 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.94301) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60371 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.15091) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21619 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.76339) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22243 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-0.76962) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37051 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.91770) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55431 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-2.10151) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56729 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-2.11449) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73826 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-2.28546) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69529 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-3.24248) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87135 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-2.41855) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77386 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-2.32105) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90629 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-2.45349) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19332 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (0.25949) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43738 HOMO: -6.61237 LUMO: -0.87076 factor:1 | -1 (0.01543) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52598 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-0.07317) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32840 HOMO: -6.97700 LUMO: 0.13061 factor:1 | -1 (0.12441) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21019 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (0.24262) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24815 HOMO: -6.86543 LUMO: -0.91430 factor:1 | -1 (0.20466) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43096 HOMO: -6.74298 LUMO: 0.28028 factor:1 | -1 (0.02185) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76321 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.31040) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50742 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.05461) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11694 HOMO: -6.86543 LUMO: 0.49253 factor:1 | -1 (0.33587) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38595 HOMO: -6.11440 LUMO: -1.12655 factor:1 | -1 (0.06686) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83576 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-2.38296) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73347 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-2.28067) | -1 | -1 |
| 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: -7.18108 LUMO: 0.00000 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: -11510.21569 HOMO: -6.86271 LUMO: -1.15376 factor:1 | -1 (0.23712) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07479 HOMO: -6.78108 LUMO: -1.22723 factor:1 | -1 (0.37802) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15536 HOMO: -6.40828 LUMO: 0.02449 factor:1 | -1 (0.29745) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26412 HOMO: -6.43821 LUMO: 0.09796 factor:1 | -1 (0.18868) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41634 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (0.03646) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89392 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.44112) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65209 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.19929) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71340 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-1.26059) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29933 HOMO: -6.60148 LUMO: -0.59865 factor:1 | -1 (0.15347) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34094 HOMO: -6.72938 LUMO: 0.30749 factor:1 | -1 (0.11187) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51708 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.06427) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37116 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-0.91836) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39111 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.93830) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59462 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.14182) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95025 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-1.49744) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60400 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-2.15120) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71667 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.26386) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74075 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.28794) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32109 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.86828) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30531 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-0.85251) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38599 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-0.93319) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54962 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.09681) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04688 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.59408) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18267 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.72986) | -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: -11511.03339 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.58058) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23734 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-0.78453) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20219 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.25062) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14728 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.30553) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34287 HOMO: -7.09673 LUMO: 0.28300 factor:1 | -1 (0.10993) | 1 | 1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29838 HOMO: -6.57155 LUMO: -1.11567 factor:1 | -1 (0.15442) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25016 HOMO: -6.38379 LUMO: -0.60681 factor:1 | -1 (0.20264) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17231 HOMO: -6.60148 LUMO: 0.18232 factor:1 | -1 (0.28049) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37501 HOMO: -6.96067 LUMO: -0.52246 factor:1 | -1 (0.07780) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26208 HOMO: -6.57427 LUMO: -0.84627 factor:1 | -1 (0.19072) | -1 | -1 |
| 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: -6.59332 LUMO: -0.98233 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: -11511.47204 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.01923) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32564 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.87283) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53849 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-1.08568) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14560 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-1.69279) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25581 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.80301) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42806 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.97526) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28436 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-0.83155) | -1 | -1 |
| G: -5246.08711 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49212 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.03931) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80934 HOMO: -6.83550 LUMO: 0.03537 factor:1 | -1 (1.20481) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33558 HOMO: -7.47769 LUMO: 0.40817 factor:1 | -1 (0.67857) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38711 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.37296) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11190 HOMO: -6.74842 LUMO: -0.16327 factor:1 | -1 (0.90225) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98311 HOMO: -7.07224 LUMO: 0.61770 factor:1 | -1 (1.03104) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98321 HOMO: -6.83006 LUMO: 0.54695 factor:1 | -1 (0.03094) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64501 HOMO: -6.60148 LUMO: 1.23540 factor:1 | -1 (1.36914) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15272 HOMO: -6.99061 LUMO: 0.41089 factor:1 | -1 (0.86143) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29212 HOMO: -6.63686 LUMO: 0.85172 factor:1 | -1 (0.72203) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89432 HOMO: -6.50624 LUMO: 0.12517 factor:1 | -1 (1.11983) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17222 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.15807) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44943 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.43527) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26383 HOMO: -6.63141 LUMO: 1.25717 factor:1 | -1 (0.75033) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91753 HOMO: -6.91441 LUMO: 1.32792 factor:1 | -1 (1.09662) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87067 HOMO: -7.15387 LUMO: 0.64219 factor:1 | -1 (1.14348) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35762 HOMO: -7.17836 LUMO: 0.60409 factor:1 | -1 (0.65653) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02564 HOMO: -6.92258 LUMO: 0.49525 factor:1 | -1 (0.98851) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23660 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.22245) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33582 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.32167) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95141 HOMO: -6.48447 LUMO: 0.37552 factor:1 | -1 (1.06274) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02889 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-1.01474) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27119 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.25704) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23652 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.22237) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43051 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.41636) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24537 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.23122) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78916 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.77501) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43111 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.41696) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55547 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.54132) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00037 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.98622) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04710 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-1.03294) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56747 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.55332) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08420 HOMO: -6.41100 LUMO: 1.39050 factor:1 | -1 (0.92995) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89051 HOMO: -5.92664 LUMO: 1.65989 factor:1 | -1 (1.12364) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09960 HOMO: -6.07630 LUMO: 1.54833 factor:1 | -1 (0.91455) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06526 HOMO: -6.45998 LUMO: 0.68573 factor:1 | -1 (0.94889) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98094 HOMO: -6.52801 LUMO: 0.41361 factor:1 | -1 (1.03322) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06746 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.05331) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84707 HOMO: -6.56339 LUMO: 1.65717 factor:1 | -1 (0.16708) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48100 HOMO: -5.85861 LUMO: 1.90752 factor:1 | -1 (0.53315) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68413 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.33002) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84648 HOMO: -6.53890 LUMO: -1.82588 factor:1 | -1 (0.16768) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08290 HOMO: -6.50352 LUMO: -1.66806 factor:1 | -1 (0.93126) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87386 HOMO: -6.90625 LUMO: 0.43538 factor:1 | -1 (1.14029) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16483 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (0.84932) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93898 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (1.07518) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11855 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (1.89560) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46201 HOMO: -5.31166 LUMO: 0.34286 factor:1 | -1 (0.55215) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59763 HOMO: -6.42461 LUMO: 0.74287 factor:1 | -1 (0.41652) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20551 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.80864) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08124 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.93292) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10184 HOMO: -6.75659 LUMO: -0.34014 factor:1 | -1 (0.91232) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75839 HOMO: -6.63958 LUMO: 0.36191 factor:1 | -1 (0.25576) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88360 HOMO: -5.92936 LUMO: -0.67484 factor:1 | -1 (1.13055) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96069 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (1.05346) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75650 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (1.25766) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20423 HOMO: -6.35930 LUMO: -0.75648 factor:1 | -1 (0.80992) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07256 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (0.94160) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84678 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (1.16737) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66912 HOMO: -6.90897 LUMO: 0.26123 factor:1 | -1 (1.34503) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67421 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (1.33994) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86069 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (1.15346) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99535 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (0.01880) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94091 HOMO: -6.52801 LUMO: 0.75376 factor:1 | -1 (1.07324) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04898 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.03483) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99790 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.98375) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20504 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-0.19089) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35895 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.34480) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.29826 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (1.71590) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.25605 HOMO: -6.30760 LUMO: -0.66668 factor:1 | -1 (1.75810) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90015 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (2.11400) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09433 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.91983) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97786 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (1.03629) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99103 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (1.02312) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09601 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (0.91814) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00319 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (1.01096) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00812 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (1.00603) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.14946 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (0.86470) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03051 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (0.98364) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25732 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (0.75683) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41517 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (0.59898) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71752 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (0.29663) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04049 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.02634) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87967 HOMO: -6.72665 LUMO: 0.32654 factor:1 | -1 (0.13448) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68657 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.67242) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35742 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.34327) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18918 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.17502) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99187 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (0.02229) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21582 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.20166) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.81531 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (2.19884) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98152 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (2.03264) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.12625 HOMO: -6.70489 LUMO: 0.19048 factor:1 | -1 (1.88790) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90044 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (1.11371) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64928 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (1.36487) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89402 HOMO: -6.77564 LUMO: 0.72382 factor:1 | -1 (1.12013) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01955 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.99460) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98722 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (1.02693) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98521 HOMO: -7.09945 LUMO: 0.33470 factor:1 | -1 (1.02894) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98189 HOMO: -7.20830 LUMO: 0.59593 factor:1 | -1 (1.03226) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04398 HOMO: -6.40556 LUMO: 0.56600 factor:1 | -1 (0.97017) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78854 HOMO: -6.77291 LUMO: 0.73471 factor:1 | -1 (0.22561) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58084 HOMO: -6.65046 LUMO: 0.09796 factor:1 | -1 (0.43331) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74575 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (1.26840) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00796 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (1.00620) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97391 HOMO: -7.27360 LUMO: 0.42178 factor:1 | -1 (0.04025) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99391 HOMO: -6.78924 LUMO: -0.13334 factor:1 | -1 (0.02025) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75863 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.74448) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24618 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.23203) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16313 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.14898) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24967 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.23551) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15021 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.13606) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48007 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.46591) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65951 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.35465) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93695 HOMO: -6.37291 LUMO: -0.67212 factor:1 | -1 (0.07720) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91287 HOMO: -6.65591 LUMO: 0.03810 factor:1 | -1 (0.10128) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35925 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.34509) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04704 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-1.03289) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29340 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.27924) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30382 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.28967) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05728 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.04313) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44817 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.43402) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79076 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.77661) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80668 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.79253) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98145 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (1.03270) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01604 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.99811) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.13084 HOMO: -6.88720 LUMO: -1.20274 factor:1 | -1 (0.88331) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05887 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (0.95528) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94251 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (1.07164) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61999 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (0.39416) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05396 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.03981) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90585 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (0.10830) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86438 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.14977) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26812 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.25396) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34447 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.33032) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97848 HOMO: -6.81645 LUMO: -0.85444 factor:1 | -1 (0.03567) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23032 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.21617) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01998 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.00582) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03481 HOMO: -6.52529 LUMO: 1.58914 factor:1 | -1 (0.97934) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88820 HOMO: -6.58516 LUMO: 1.97555 factor:1 | -1 (1.12595) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01136 HOMO: -6.84366 LUMO: 0.15783 factor:1 | -1 (1.00279) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86787 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (1.14628) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15797 HOMO: -6.75387 LUMO: 0.14422 factor:1 | -1 (0.85618) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07990 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (0.93425) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79816 HOMO: -6.59876 LUMO: 1.90208 factor:1 | -1 (1.21600) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.69633 HOMO: -7.05863 LUMO: 1.20819 factor:1 | -1 (1.31782) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07343 HOMO: -6.54978 LUMO: 2.01636 factor:1 | -1 (0.94072) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90896 HOMO: -5.52119 LUMO: 1.95106 factor:1 | -1 (1.10519) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99190 HOMO: -6.53617 LUMO: 1.60275 factor:1 | -1 (1.02225) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70547 HOMO: -6.11440 LUMO: 1.89119 factor:1 | -1 (0.30869) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77573 HOMO: -7.31986 LUMO: 0.48708 factor:1 | -1 (0.23843) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69267 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.67852) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28885 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.27470) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76669 HOMO: -6.87087 LUMO: 0.72927 factor:1 | -1 (0.24746) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08234 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.06819) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98338 HOMO: -6.54706 LUMO: -0.03265 factor:1 | -1 (0.03078) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34431 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.33016) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79442 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (0.21973) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88408 HOMO: -7.04503 LUMO: -0.10068 factor:1 | -1 (0.13007) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73864 HOMO: -6.67223 LUMO: 0.03537 factor:1 | -1 (0.27552) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66272 HOMO: -6.82734 LUMO: 0.58777 factor:1 | -1 (0.35144) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56742 HOMO: -6.84366 LUMO: 0.46531 factor:1 | -1 (0.44673) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92020 HOMO: -7.03959 LUMO: -1.15104 factor:1 | -1 (1.09395) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62907 HOMO: -6.91169 LUMO: -0.41361 factor:1 | -1 (1.38509) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93503 HOMO: -7.10217 LUMO: -0.44627 factor:1 | -1 (1.07912) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99979 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (1.01436) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11090 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.90325) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19308 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.82108) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45773 HOMO: -6.71305 LUMO: -0.13061 factor:1 | -1 (0.55642) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67972 HOMO: -6.74842 LUMO: -0.36191 factor:1 | -1 (0.33443) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46184 HOMO: -6.74570 LUMO: -0.09796 factor:1 | -1 (0.55231) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71982 HOMO: -6.93890 LUMO: -0.27211 factor:1 | -1 (1.29434) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88785 HOMO: -6.88720 LUMO: -0.18776 factor:1 | -1 (1.12631) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97253 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (1.04162) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91813 HOMO: -6.70216 LUMO: 0.01361 factor:1 | -1 (1.09602) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87965 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (1.13450) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88278 HOMO: -6.18243 LUMO: 0.25851 factor:1 | -1 (0.13138) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81502 HOMO: -6.32937 LUMO: -0.20953 factor:1 | -1 (0.19913) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81224 HOMO: -6.78108 LUMO: 0.00544 factor:1 | -1 (0.20191) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60010 HOMO: -5.97562 LUMO: 0.28572 factor:1 | -1 (0.41405) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82261 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (0.19154) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25855 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.75561) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41705 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (0.59710) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01217 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (1.00198) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03245 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (0.98171) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30154 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (0.71261) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84920 HOMO: -6.90081 LUMO: -0.20136 factor:1 | -1 (0.16496) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81997 HOMO: -7.12938 LUMO: -0.25851 factor:1 | -1 (0.19418) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89540 HOMO: -6.93074 LUMO: -0.26667 factor:1 | -1 (0.11875) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41297 HOMO: -7.00421 LUMO: -0.31021 factor:1 | -1 (0.60118) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18558 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.17143) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28550 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.27135) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13410 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.11995) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.53982 HOMO: -6.80829 LUMO: -0.29933 factor:1 | -1 (2.47433) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.82105 HOMO: -6.84094 LUMO: -0.53606 factor:1 | -1 (2.19310) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.83128 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (2.18287) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88066 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (1.13349) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78221 HOMO: -6.39468 LUMO: -1.06941 factor:1 | -1 (1.23194) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64754 HOMO: -6.00827 LUMO: -1.94017 factor:1 | -1 (1.36661) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91202 HOMO: -6.80829 LUMO: 0.18504 factor:1 | -1 (2.10213) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59402 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (1.42014) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32056 HOMO: -6.45454 LUMO: -0.07347 factor:1 | -1 (0.69359) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22336 HOMO: -5.33887 LUMO: 1.11839 factor:1 | -1 (0.79079) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39692 HOMO: -5.75249 LUMO: 0.70477 factor:1 | -1 (0.61724) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88375 HOMO: -5.64092 LUMO: 0.87076 factor:1 | -1 (0.13040) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68775 HOMO: -5.14295 LUMO: 1.06124 factor:1 | -1 (0.32640) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78637 HOMO: -5.05043 LUMO: 1.21091 factor:1 | -1 (0.22779) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64974 HOMO: -5.05588 LUMO: 1.02859 factor:1 | -1 (0.36441) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63736 HOMO: -5.76337 LUMO: 0.79457 factor:1 | -1 (1.37679) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78243 HOMO: -5.01506 LUMO: 1.00138 factor:1 | -1 (1.23172) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64544 HOMO: -4.84363 LUMO: 1.53744 factor:1 | -1 (0.36871) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65923 HOMO: -5.17833 LUMO: 1.45309 factor:1 | -1 (0.35492) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72065 HOMO: -5.13751 LUMO: 0.51157 factor:1 | -1 (0.29350) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53178 HOMO: -5.56473 LUMO: 0.32109 factor:1 | -1 (0.48238) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81706 HOMO: -4.69941 LUMO: 1.14016 factor:1 | -1 (0.19709) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88536 HOMO: -4.49260 LUMO: 1.86398 factor:1 | -1 (0.12879) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59665 HOMO: -4.32117 LUMO: 1.68438 factor:1 | -1 (0.41750) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49194 HOMO: -4.44906 LUMO: 1.37690 factor:1 | -1 (0.52221) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02575 HOMO: -4.62049 LUMO: 1.34968 factor:1 | -1 (0.98840) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93742 HOMO: -4.59600 LUMO: 1.58370 factor:1 | -1 (1.07673) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.96075 HOMO: -4.98785 LUMO: 1.46669 factor:1 | -1 (2.05340) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91380 HOMO: -5.06676 LUMO: 1.27349 factor:1 | -1 (1.10035) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24600 HOMO: -5.09125 LUMO: 1.13471 factor:1 | -1 (0.76815) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66104 HOMO: -4.84635 LUMO: 1.33608 factor:1 | -1 (1.35311) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61785 HOMO: -4.94431 LUMO: 1.18370 factor:1 | -1 (1.39630) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87914 HOMO: -4.92526 LUMO: 1.39867 factor:1 | -1 (1.13501) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86648 HOMO: -5.71983 LUMO: 0.60137 factor:1 | -1 (1.14767) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76335 HOMO: -5.10486 LUMO: 1.05580 factor:1 | -1 (1.25080) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00627 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-1.99212) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01060 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.99644) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03384 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-2.01968) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23008 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-2.21593) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79247 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-1.77832) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11740 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-2.10325) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66477 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.65062) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88406 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.86991) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27012 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-1.25597) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27408 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-2.25993) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21520 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-2.20105) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77484 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-1.76069) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05933 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-2.04518) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21360 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.19945) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30777 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-2.29362) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48956 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.47541) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63824 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-1.62408) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88899 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.87484) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20026 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-2.18611) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29162 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.27747) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38976 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-2.37561) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48454 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-2.47039) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81405 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-1.79990) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99680 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.98265) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26339 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-2.24924) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31738 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-2.30323) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.91850 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-2.90435) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86736 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.85320) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.84419 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-2.83004) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27400 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-2.25985) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15786 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-2.14371) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90006 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-1.88591) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28821 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-2.27406) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72082 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-1.70667) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63127 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.61712) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72493 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.71078) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49557 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.48142) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67877 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-2.66462) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53195 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-1.51780) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88975 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.87560) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12010 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-2.10594) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97212 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.95797) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05525 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.04110) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90627 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.89212) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96537 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.95122) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98262 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-1.96847) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96230 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.94814) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07043 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-2.05628) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10001 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-2.08586) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06826 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-2.05411) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13201 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-2.11786) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08301 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-2.06885) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11003 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-2.09588) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.09900 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-3.08485) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84012 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.82597) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91258 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.89843) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95367 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.93952) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82926 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.81511) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86270 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.84855) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76613 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.75198) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01852 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-2.00436) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85802 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.84387) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91726 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.90311) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92292 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.90877) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03220 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-2.01805) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64610 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.63195) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67786 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.66370) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79691 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-1.78275) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82907 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.81492) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94692 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.93277) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63663 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-1.62248) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76831 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.75415) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59552 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.58137) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82904 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.81489) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63786 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-1.62370) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92763 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-1.91348) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88877 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-1.87462) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69892 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-1.68477) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85663 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-1.84248) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55282 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.53867) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51973 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.50558) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52746 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.51331) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60082 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.58667) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45815 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.44400) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57709 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-1.56294) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85917 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.84501) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41527 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.40111) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51624 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-2.50209) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99490 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.98074) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84017 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.82602) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80621 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.79206) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05816 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-2.04401) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.97843) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33169 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-2.31754) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61042 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-2.59627) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87655 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-1.86240) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98349 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-1.96934) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56895 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-2.55480) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74714 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.73298) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60531 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.59116) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62964 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.61549) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67290 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.65875) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16203 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-2.14788) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55138 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.53723) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61617 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-1.60202) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69397 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-1.67981) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34340 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.32925) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.13162 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-3.11747) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15435 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-2.14020) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.12093 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-3.10678) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82768 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.81353) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78371 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-1.76956) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89868 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.88452) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99043 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.97628) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90281 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.88866) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10377 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-2.08962) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37550 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-2.36135) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52854 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-2.51439) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92997 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-1.91582) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96336 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-1.94921) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90107 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.88692) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61617 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.60202) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70637 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.69222) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26793 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-2.25378) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59034 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.57619) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52125 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-1.50710) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65181 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-1.63766) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79633 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-1.78218) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74648 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-1.73233) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98216 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.96801) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04638 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-2.03223) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79884 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.78469) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88836 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.87421) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74934 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.73519) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90698 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-1.89282) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49742 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-1.48327) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59062 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.57646) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38838 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-1.37423) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41796 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.40381) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59459 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-1.58044) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02281 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-2.00866) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99680 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-1.98265) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90981 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-1.89565) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81380 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.79965) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45875 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.44460) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33159 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.31744) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05994 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-1.04579) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07874 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-1.06459) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40751 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-1.39336) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42672 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-1.41257) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12002 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-1.10587) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59848 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-1.58433) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38747 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-2.37332) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74915 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-1.73500) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81002 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.79587) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98126 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.96711) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-1.99759) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56413 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-2.54998) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81427 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-1.80011) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79163 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-1.77747) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91098 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-1.89682) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56881 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-2.55466) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69190 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.67775) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69026 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.67611) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70335 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.68920) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73489 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.72074) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60501 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.59086) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76798 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.75383) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35264 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-2.33849) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52188 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-1.50773) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46817 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.45401) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88887 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-2.87472) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71250 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.69834) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44789 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-1.43374) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57165 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.55750) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35273 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.33858) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09438 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-2.08023) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97051 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.95636) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08012 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-2.06597) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97653 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.96238) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38746 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-1.37330) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18767 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-1.17352) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31235 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-1.29820) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20865 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-1.19450) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50980 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-1.49565) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18944 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-1.17529) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43859 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-1.42443) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73473 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.72058) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78480 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-1.77064) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53644 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.52229) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14848 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-2.13433) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11435 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-2.10020) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08434 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-2.07019) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91530 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.90115) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48558 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.47143) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27472 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-1.26057) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43393 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-1.41978) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33399 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-1.31983) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70896 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-1.69481) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77853 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-2.76438) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66338 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-1.64923) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70450 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-1.69034) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80687 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-1.79271) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83870 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-1.82455) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86687 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.85271) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04387 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.02971) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86483 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-1.85067) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68711 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.67296) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71089 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-1.69674) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66387 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-1.64972) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73163 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.71747) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45002 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.43586) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55342 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-1.53927) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70618 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-1.69203) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22593 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-1.21178) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00620 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.99205) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38226 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-1.36811) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06503 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-1.05088) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56980 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-1.55565) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89007 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-2.87592) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86156 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-1.84741) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70319 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-1.68904) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79484 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-1.78069) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96746 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-2.95331) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74205 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.72790) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77013 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-1.75598) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06886 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-2.05470) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23359 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-2.21944) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42509 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.41094) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99201 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-1.97786) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44245 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-1.42830) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57113 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.55698) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32528 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.31113) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75454 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.74039) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27330 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-1.25915) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51608 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-1.50193) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57189 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-1.55774) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76112 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-1.74697) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08872 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-2.07457) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43165 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.41750) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07563 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-2.06148) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41480 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.40065) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61652 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-1.60237) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55462 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.54046) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82001 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-1.80586) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40090 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-1.38675) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64629 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-1.63214) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66455 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.65040) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84526 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-1.83111) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99552 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.98137) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14543 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-2.13128) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30257 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-2.28842) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50468 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-1.49053) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52602 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-1.51186) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69383 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-1.67968) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14644 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-2.13228) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01543 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.00128) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22941 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-1.21526) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49848 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-1.48433) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78425 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.77010) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53745 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-1.52329) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03949 HOMO: -5.95657 LUMO: 0.37552 factor:1 | -1 (0.97466) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72847 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-1.71432) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20249 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-2.18834) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18089 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-2.16673) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38913 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-2.37498) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65459 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-1.64044) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66047 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.64632) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09386 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-2.07971) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27876 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-2.26461) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96981 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-1.95566) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43045 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-1.41630) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60384 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-1.58969) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86991 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-1.85576) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85712 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-1.84297) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70931 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-1.69516) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42019 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.40604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81987 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-1.80572) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.91448 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-2.90033) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86357 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-1.84942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.84762 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-2.83347) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16399 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-2.14984) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26440 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-2.25025) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70009 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.68594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14325 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-2.12910) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53750 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-1.52335) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92344 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.90929) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55750 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-1.54335) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89005 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.87590) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35940 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-1.34525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61538 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-1.60123) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10750 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-2.09334) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78126 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-1.76711) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59127 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.57712) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33260 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-1.31845) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36732 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-1.35317) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44229 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.42814) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15314 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-1.13899) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46980 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-1.45565) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62708 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.61293) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85976 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-1.84561) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52085 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-1.50669) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62898 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-1.61483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67434 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-2.66019) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46104 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-1.44688) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76058 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-1.74643) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99400 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.97985) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67666 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-1.66251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71742 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.70327) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64286 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-1.62871) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70882 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-1.69467) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82790 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-1.81375) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88232 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-1.86817) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38384 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-1.36969) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54934 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.53518) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78697 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-1.77282) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69402 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-1.67987) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60896 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-1.59480) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78569 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-1.77154) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22256 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-1.20840) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46898 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-1.45483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17319 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-1.15904) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98356 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.96941) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24781 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-1.23366) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97624 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.96209) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96029 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.94614) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10212 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-1.08797) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53802 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-1.52386) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30960 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-1.29545) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42046 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-1.40631) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63078 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-1.61663) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47461 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-1.46046) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58376 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-1.56961) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44550 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-1.43135) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01656 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-1.00241) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48627 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.47212) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31108 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.29693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22428 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.21013) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46896 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.45481) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30314 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.28898) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88976 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.87561) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75898 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.74483) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81702 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.80287) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70510 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.69095) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11290 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.09875) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.69244 HOMO: -5.97562 LUMO: 1.42316 factor:1 | -1 (1.32171) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16874 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.15459) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17135 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.15720) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98972 HOMO: -7.40966 LUMO: 0.19592 factor:1 | -1 (0.02444) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06836 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.05421) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11873 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.10457) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05981 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.04566) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94814 HOMO: -6.99333 LUMO: -1.65717 factor:1 | -1 (0.06601) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15775 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.14359) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40296 HOMO: -6.87904 LUMO: -1.79323 factor:1 | -1 (0.61119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20733 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (0.80682) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28973 HOMO: -7.13210 LUMO: -1.17553 factor:1 | -1 (0.72442) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26668 HOMO: -6.52801 LUMO: -2.23678 factor:1 | -1 (0.74747) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59799 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (1.41616) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35683 HOMO: -7.30626 LUMO: -1.66806 factor:1 | -1 (0.65732) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55383 HOMO: -6.98516 LUMO: -1.40683 factor:1 | -1 (1.46033) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.27061 HOMO: -6.95523 LUMO: -0.97145 factor:1 | -1 (1.74354) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28559 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.27143) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74617 HOMO: -7.25456 LUMO: -2.97420 factor:1 | -1 (0.26798) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44179 HOMO: -6.80557 LUMO: -2.65039 factor:1 | -1 (0.57236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51627 HOMO: -7.10489 LUMO: 0.77008 factor:1 | -1 (0.49789) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98073 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.96658) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55473 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.54058) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15383 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.13968) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14654 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.13238) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51914 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.50499) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48254 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.46839) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08311 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.06895) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40200 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-0.38784) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69055 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-0.67639) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57716 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.56300) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39150 HOMO: -6.93890 LUMO: -2.65039 factor:1 | -1 (0.62265) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30009 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.28594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46970 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.45555) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64723 HOMO: -7.01782 LUMO: -1.09662 factor:1 | -1 (0.36692) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49050 HOMO: -6.58516 LUMO: -0.83539 factor:1 | -1 (0.52366) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60035 HOMO: -7.46953 LUMO: 0.06259 factor:1 | -1 (0.41380) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58623 HOMO: -6.96884 LUMO: -0.99866 factor:1 | -1 (0.42793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91578 HOMO: -7.29809 LUMO: -0.19320 factor:1 | -1 (0.09837) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67064 HOMO: -6.86271 LUMO: 0.04082 factor:1 | -1 (0.34352) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05345 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.03929) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54876 HOMO: -7.15659 LUMO: -1.25989 factor:1 | -1 (0.46540) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56069 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.54654) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13317 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.11902) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19203 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.17788) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18848 HOMO: -6.93346 LUMO: -0.87349 factor:1 | -1 (0.82568) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33632 HOMO: -6.77019 LUMO: -0.87349 factor:1 | -1 (0.67784) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46992 HOMO: -6.59060 LUMO: -0.82995 factor:1 | -1 (0.54423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.28422) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96729 HOMO: -7.27088 LUMO: -1.18642 factor:1 | -1 (0.04686) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26450 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-0.25034) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24561 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.23146) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02313 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.00898) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12908 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.11493) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15513 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.14097) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22724 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.21308) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84530 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.83114) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83762 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.82347) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81025 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.79610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66464 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.65049) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78842 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.77427) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62230 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-0.60815) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11785 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.10370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27485 HOMO: -7.00965 LUMO: -1.37690 factor:1 | -1 (0.73931) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27368 HOMO: -6.97972 LUMO: -1.58098 factor:1 | -1 (0.74048) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25068 HOMO: -6.91169 LUMO: -1.48574 factor:1 | -1 (0.76347) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81630 HOMO: -6.90081 LUMO: -1.30343 factor:1 | -1 (0.19785) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08923 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.07508) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27016 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.25600) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26112 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.24697) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75744 HOMO: -7.16204 LUMO: -1.30070 factor:1 | -1 (0.25671) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86493 HOMO: -7.32803 LUMO: 0.14694 factor:1 | -1 (1.14922) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89405 HOMO: -6.99877 LUMO: -0.87621 factor:1 | -1 (1.12010) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60201 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (0.41214) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43794 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.42379) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51235 HOMO: -6.90897 LUMO: -1.14016 factor:1 | -1 (0.50181) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60040 HOMO: -6.68312 LUMO: -0.74831 factor:1 | -1 (0.41375) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56530 HOMO: -6.99061 LUMO: -0.86804 factor:1 | -1 (0.44885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53435 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.52020) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48412 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-0.46997) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58646 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.57231) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80368 HOMO: -7.01510 LUMO: -0.99322 factor:1 | -1 (1.21047) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73625 HOMO: -6.88720 LUMO: -0.87893 factor:1 | -1 (1.27790) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39074 HOMO: -6.88448 LUMO: 0.22041 factor:1 | -1 (0.62341) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59719 HOMO: -7.55932 LUMO: 1.12111 factor:1 | -1 (0.41696) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61877 HOMO: -6.46815 LUMO: -0.86260 factor:1 | -1 (0.39538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80115 HOMO: -7.13755 LUMO: 0.23130 factor:1 | -1 (1.21300) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78387 HOMO: -6.78924 LUMO: 1.51023 factor:1 | -1 (1.23028) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80033 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (1.21382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74758 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.73343) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98230 HOMO: -6.49536 LUMO: 1.70615 factor:1 | -1 (1.03186) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80847 HOMO: -6.38651 LUMO: 1.44492 factor:1 | -1 (1.20568) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72229 HOMO: -6.83822 LUMO: 1.38234 factor:1 | -1 (1.29186) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77105 HOMO: -6.01644 LUMO: 1.20274 factor:1 | -1 (1.24310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71160 HOMO: -6.18243 LUMO: 1.77962 factor:1 | -1 (1.30255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40843 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (0.60573) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78471 HOMO: -6.61237 LUMO: -0.91702 factor:1 | -1 (1.22944) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70474 HOMO: -6.84094 LUMO: -0.84900 factor:1 | -1 (1.30941) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80096 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (1.21319) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78499 HOMO: -7.86953 LUMO: 1.16737 factor:1 | -1 (1.22917) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58544 HOMO: -7.40694 LUMO: 0.11429 factor:1 | -1 (0.42872) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52369 HOMO: -6.70489 LUMO: -0.65035 factor:1 | -1 (0.49046) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66265 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.64850) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58048 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.56632) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65259 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.63843) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78064 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.76649) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76431 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (1.24985) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75762 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.74347) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74271 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.72856) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58665 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.57250) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70426 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.69011) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.92326 HOMO: -7.36884 LUMO: 0.38096 factor:1 | -1 (3.09089) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.76623 HOMO: -6.99333 LUMO: 1.74153 factor:1 | -1 (3.24792) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84227 HOMO: -6.94435 LUMO: 1.74969 factor:1 | -1 (1.17189) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15816 HOMO: -7.02598 LUMO: 1.43404 factor:1 | -1 (0.85599) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63284 HOMO: -6.41100 LUMO: 1.62996 factor:1 | -1 (0.38131) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50647 HOMO: -6.57699 LUMO: 1.81228 factor:1 | -1 (0.50768) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50952 HOMO: -6.86543 LUMO: 1.49935 factor:1 | -1 (0.50464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57098 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.55683) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53598 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-0.52183) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56380 HOMO: -7.48857 LUMO: 0.10340 factor:1 | -1 (0.45035) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54232 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.52817) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68331 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.66916) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55103 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-0.53688) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59671 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.58256) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47935 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-1.46520) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28335 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.26919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18451 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-1.17036) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70958 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-1.69543) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50871 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34256 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.32841) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24022 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.22606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15262 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.13847) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47593 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.46178) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45310 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.43895) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41838 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.40423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49350 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-1.47935) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80432 HOMO: -6.50624 LUMO: -0.70477 factor:1 | -1 (0.20983) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80944 HOMO: -7.35524 LUMO: 0.75103 factor:1 | -1 (0.20471) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27748 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.26332) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15233 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.13818) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15496 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-1.14081) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10563 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-1.09148) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16109 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.14694) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42871 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-1.41456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54893 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.53478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45943 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-1.44528) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31450 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-1.30035) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51701 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-1.50286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89745 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-1.88330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44397 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-1.42982) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44050 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.42635) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26409 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.24994) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01034 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (0.00381) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01470 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.00054) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60766 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.59351) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19704 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.18289) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87902 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.13513) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09848 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-0.08433) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29571 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-0.28156) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62634 HOMO: -6.58243 LUMO: -0.48980 factor:1 | -1 (0.38782) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76268 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-0.74853) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73544 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-0.72129) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75125 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.73710) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72184 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.70769) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16650 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-1.15235) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28207 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.26791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49375 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.47960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32676 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.31260) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05926 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.04511) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92960 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.91545) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84792 HOMO: -7.07224 LUMO: -1.08573 factor:1 | -1 (0.16623) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39598 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.38183) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02911 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.01496) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82796 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-0.81381) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86294 HOMO: -6.85183 LUMO: -0.68573 factor:1 | -1 (0.15121) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17417 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-1.16002) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74466 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.73051) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87119 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.85704) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62169 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-1.60754) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58942 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.57527) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96635 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.95220) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47886 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.46471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00122 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.98707) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24010 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-2.22595) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16113 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-2.14698) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26298 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-2.24883) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65347 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.63932) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93051 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.91636) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85304 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-1.83889) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91734 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.90319) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40048 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.38633) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95217 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-1.93802) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83091 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.81676) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86368 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.84953) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62656 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.61241) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38457 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.37042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24693 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-2.23278) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17305 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-2.15890) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06690 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-2.05275) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75612 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.74196) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90466 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.89051) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23142 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-2.21727) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47918 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-2.46503) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58718 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-2.57303) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.12009 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-3.10593) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04544 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.03128) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08476 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.07060) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08168 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.06753) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65192 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.63777) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82358 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-0.80943) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54094 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-0.52679) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62264 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.60849) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66006 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.64591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64218 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.62803) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74107 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.72692) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89977 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.88562) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01994 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.00579) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02046 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.00630) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26022 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.24606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62248 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.60833) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44830 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.43415) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33829 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.32413) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70806 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.69391) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60724 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-1.59309) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73890 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.72475) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67327 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.65911) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03022 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-2.01606) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13577 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-2.12162) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11042 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.09627) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00807 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.99392) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83161 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.81746) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77990 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.76575) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67927 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.66512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77745 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.76330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36210 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.34795) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20795 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.19380) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85490 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.84075) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12888 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.11472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95295 HOMO: -7.48585 LUMO: 0.05987 factor:1 | -1 (0.06120) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02666 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-1.01251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88834 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.87419) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78377 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.76962) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26863 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.25448) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06980 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.05565) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94962 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-0.93547) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08749 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.07333) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81322 HOMO: -6.43277 LUMO: -1.07485 factor:1 | -1 (0.20093) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93681 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.92266) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72965 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-0.71550) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86720 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-0.85305) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68894 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.67479) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73958 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.72543) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91262 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.89847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71215 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-0.69800) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95436 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.94021) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39799 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-1.38384) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68746 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-1.67331) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36536 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.35121) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52879 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.51464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98227 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.96812) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11447 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.10032) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89874 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-0.88459) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07295 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.05880) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44016 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-1.42601) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84526 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-1.83111) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62126 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-1.60710) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73873 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.72458) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82184 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.80769) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23223 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-2.21808) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31047 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-2.29631) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78856 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.77441) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52080 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.50665) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79683 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.78268) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63813 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-1.62398) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88481 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.87066) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85694 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.84279) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13428 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-1.12013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26672 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-1.25257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14950 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.13535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74450 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-1.73034) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82736 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-1.81320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65084 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.63669) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50148 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.48733) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66557 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.65141) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19164 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-1.17749) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49478 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-1.48063) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01218 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.99803) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18710 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-1.17295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45800 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.44384) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34133 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-1.32718) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70093 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-1.68678) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57554 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-1.56139) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59775 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-1.58359) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47276 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-1.45861) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36985 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-1.35570) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38307 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-2.36891) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38922 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-2.37506) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24206 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-2.22791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09691 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-2.08276) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06039 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-2.04624) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87509 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.86094) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89858 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.88442) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04008 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-1.02592) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87327 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.85912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16849 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.15433) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65922 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.64506) | 1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66847 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.65432) | 1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73250 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-1.71834) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32577 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.31162) | 1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48270 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.46854) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85749 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.84334) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65437 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-1.64022) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11479 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-2.10064) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10159 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-2.08744) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60343 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-1.58928) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64923 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.63508) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80091 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.78675) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45312 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-1.43897) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45739 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.44324) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35052 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-2.33637) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38366 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-2.36951) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53662 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-2.52247) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78076 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-2.76661) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20578 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-2.19163) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87400 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-1.85984) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81576 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.80161) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86589 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-1.85173) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65640 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-2.64225) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77265 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-2.75850) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06767 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-1.05352) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91724 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.90309) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19034 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-1.17618) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78510 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.77095) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81819 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-0.80404) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78964 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.77549) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64166 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.62751) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65571 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.64155) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91251 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.89836) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92440 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.91025) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76486 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-0.75071) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69789 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.68374) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59267 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.57851) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39987 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.38572) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66556 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.65140) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42280 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-1.40865) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27320 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-1.25904) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92464 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-1.91048) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94660 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.93245) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95928 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.94513) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58080 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-0.56665) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05923 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-1.04508) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46963 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-1.45548) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79394 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.77979) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36493 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.35077) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81697 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.80282) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47233 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.45818) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68698 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-0.67283) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02630 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-2.01215) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08382 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-2.06967) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79844 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.78429) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75226 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-0.73811) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78837 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-0.77422) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48735 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.47320) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15711 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.14296) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81321 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.79906) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70502 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.69087) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68616 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.67201) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43740 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.42325) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28014 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.26599) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68026 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.66611) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97738 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.96323) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16359 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-1.14944) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49502 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.48087) | 1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42112 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.40696) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87830 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.86415) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93626 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.92211) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67454 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-0.66039) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23115 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.21700) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19206 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.17791) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52238 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.50823) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54438 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-1.53023) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50648 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.49233) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71387 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.69971) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90279 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.88864) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00614 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.99199) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67196 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.65781) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74900 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.73484) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57808 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.56393) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74723 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.73307) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38939 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.37524) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51508 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.50093) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70011 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.68596) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96257 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-1.94842) | 1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35793 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.34378) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33355 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.31940) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37065 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.35650) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88984 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.87569) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28462 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-1.27047) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43646 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.42231) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30076 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.28661) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30286 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-1.28870) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99345 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-1.97930) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96651 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.95236) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83919 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.82504) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45199 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-2.43784) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.25522 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-3.24107) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74928 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-2.73513) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93454 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.92039) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86203 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.84788) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79923 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.78508) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93918 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.92502) | -1 | -1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81335 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.79920) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93994 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.92579) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78932 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.77517) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88263 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.86848) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72251 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-1.70836) | 1 | 1 |
| G: -5683.64846 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65984 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.64569) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60798 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-1.59383) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48596 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.47181) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76927 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.75512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48997 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.47582) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83234 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.81819) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07945 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.06530) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73291 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.71876) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46964 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.45549) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95945 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.94530) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39544 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.38129) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22284 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.20868) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48953 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.47537) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35075 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.33660) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37796 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.36381) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22745 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.21330) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94984 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.93569) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91335 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.89920) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99838 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.98423) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34822 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.33407) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60183 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.58768) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68177 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.66762) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12342 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-2.10926) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57549 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.56133) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49695 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-2.48279) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48253 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.46838) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64248 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.62833) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67471 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.66056) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06865 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.05450) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84614 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.83199) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56019 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.54604) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54392 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.52977) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34040 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-2.32625) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60249 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.58834) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84632 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.83217) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62415 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.61000) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73290 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.71875) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56854 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.44561) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39724 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.61691) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44453 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.43038) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00227 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-1.98812) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47753 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.46338) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63803 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.62388) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67141 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.65726) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94814 HOMO: -6.84911 LUMO: 1.98099 factor:1 | -1 (0.06601) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79932 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.21483) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89148 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.12267) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57534 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.43881) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75793 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.25622) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56876 HOMO: -6.93618 LUMO: 2.00004 factor:1 | -1 (0.44540) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36837 HOMO: -6.50896 LUMO: 1.73609 factor:1 | -1 (0.64578) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43824 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.42409) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94746 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.06670) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45226 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.43810) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75836 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.74420) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39187 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.37772) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64823 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.63408) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70399 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.68984) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44621 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.43205) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49657 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.48242) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89105 HOMO: -7.20285 LUMO: -0.66124 factor:1 | -1 (0.12310) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97605 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.96190) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19859 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.18444) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87719 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.86304) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80639 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.20776) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54758 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.53342) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53220 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.51805) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83210 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.81795) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48650 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (0.52766) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85649 HOMO: -6.67495 LUMO: 2.04358 factor:1 | -1 (0.15766) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73303 HOMO: -6.94162 LUMO: 1.73881 factor:1 | -1 (0.28112) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15576 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.14161) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94373 HOMO: -6.70489 LUMO: 2.04358 factor:1 | -1 (0.07042) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49338 HOMO: -7.04231 LUMO: 1.79323 factor:1 | -1 (0.52077) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81053 HOMO: -6.68584 LUMO: 1.60275 factor:1 | -1 (0.20362) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54941 HOMO: -6.40556 LUMO: 1.45581 factor:1 | -1 (0.46474) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11464 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.10049) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94019 HOMO: -6.84911 LUMO: 1.89935 factor:1 | -1 (0.07396) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74312 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.72897) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55256 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.53840) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92865 HOMO: -7.03686 LUMO: 2.12249 factor:1 | -1 (0.08550) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32773 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.31358) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79693 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.78278) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39845 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.38430) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65610 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.64194) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23423 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.22008) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44944 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.43529) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78686 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.77271) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76292 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.74877) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59559 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-2.58144) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.64898 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-2.63482) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24129 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-2.22714) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98838 HOMO: -7.20013 LUMO: 0.55239 factor:1 | -1 (0.02577) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60521 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.59106) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73651 HOMO: -6.69128 LUMO: -0.30477 factor:1 | -1 (0.27764) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53678 HOMO: -6.65591 LUMO: -0.25579 factor:1 | -1 (0.47737) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56698 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.55283) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38216 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.36801) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36550 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.35134) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89282 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.12134) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43294 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.41878) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51245 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.49829) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25323 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.23908) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21568 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.20153) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50422 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.49007) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47298 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.45883) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28422 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.27006) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83625 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.82210) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79416 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.78001) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84904 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.83489) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68704 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-2.67289) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65586 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-2.64171) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73579 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.72164) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56936 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-2.55520) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42191 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.40776) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40175 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.38760) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27447 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-2.26031) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14308 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.12893) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46069 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.44654) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51786 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.50371) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14961 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.13546) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11458 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.10043) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39023 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.37608) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31711 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.30296) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84232 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.82817) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67926 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.66511) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20896 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.19481) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77870 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.76455) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79064 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.77649) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44131 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.42716) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60210 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.58795) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61317 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.59902) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72349 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.70934) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96938 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.95523) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74202 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.72787) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15582 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-2.14167) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39905 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.38490) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94527 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.93112) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66605 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.65189) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86146 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.84731) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71240 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.69824) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73636 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.72221) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06486 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-2.05070) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62132 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.60717) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48695 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.47280) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37484 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.36069) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23164 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.21749) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62237 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.60822) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58405 HOMO: -6.78380 LUMO: -0.67756 factor:1 | -1 (0.43010) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76672 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.24743) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77404 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.24011) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56075 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.54660) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15301 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.13886) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71408 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.69993) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55255 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.53840) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77193 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.75778) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79566 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.78151) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61377 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.59962) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13810 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.12395) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01575 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.00160) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56447 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.55032) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48627 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.47212) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37780 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.36365) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64736 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.63321) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35595 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.34179) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24539 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.23123) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83513 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.17902) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79638 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (0.21777) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80223 HOMO: -6.88992 LUMO: 1.65173 factor:1 | -1 (0.21192) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66668 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.65253) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84929 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.83514) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88284 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.86869) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89805 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-1.88390) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42211 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.40796) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03159 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.01744) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35511 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.34096) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84478 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.83063) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10715 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.09300) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27184 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.25769) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36042 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.34626) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25519 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.24104) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23322 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.21907) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36373 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.34958) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86690 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.85275) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54136 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.52721) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60396 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.58981) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68926 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.67511) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71529 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.29886) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59491 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.41925) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74239 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (0.27176) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48546 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (0.52869) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59482 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.58066) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44915 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.43500) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66971 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.34444) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73572 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (0.27843) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78936 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (0.22479) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47175 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (0.54240) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60712 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.59296) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87907 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (0.13508) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67542 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.66126) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53426 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.52011) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42806 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.41391) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75183 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.73767) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96169 HOMO: -7.14299 LUMO: -0.63947 factor:1 | -1 (0.05246) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63583 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (0.37832) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81561 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.80146) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50839 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.49424) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19282 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.17867) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40333 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.38918) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13591 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.12176) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51990 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.50575) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75302 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.73887) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68374 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.66959) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39198 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.37783) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67875 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.66460) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16612 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.15197) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73934 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (0.27481) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79853 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (0.21562) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74324 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (0.27092) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52206 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (0.49209) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72105 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.70690) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64312 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.62896) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22235 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.20819) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91166 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.89750) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99462 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.98047) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91443 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.90028) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77892 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.76477) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78310 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-2.76895) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63651 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-2.62236) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49203 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.47788) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.75279 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-2.73864) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99282 HOMO: -6.61781 LUMO: 2.13881 factor:1 | -1 (0.02133) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79333 HOMO: -6.62597 LUMO: 2.00276 factor:1 | -1 (0.22082) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77975 HOMO: -7.01237 LUMO: 1.95922 factor:1 | -1 (0.23440) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80622 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.79207) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68037 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.66622) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52167 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.50752) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81550 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.80135) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53655 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.52240) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65724 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.64309) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64224 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.62808) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68614 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.67199) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38551 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.37135) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75784 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.74369) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55884 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.54469) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62956 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.61540) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25858 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.24443) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24636 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.23221) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14585 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.13169) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70248 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.68833) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59834 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.58419) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93495 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.92080) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80371 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.78956) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66174 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-2.64759) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74428 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.73013) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61142 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-2.59727) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77701 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-2.76285) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86380 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.84965) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07779 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.06364) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67786 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.66370) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72885 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.71470) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86289 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.84874) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30250 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.28835) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57046 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.55631) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15493 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.14078) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00116 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.98701) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12873 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.11458) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30136 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.28721) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88012 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.86597) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08886 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-2.07470) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89479 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.88064) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84470 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.83055) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75985 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.74570) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86428 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.85013) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92899 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (1.08516) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74240 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (1.27175) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87826 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.13589) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25561 HOMO: -6.67767 LUMO: -0.48436 factor:1 | -1 (0.75854) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55776 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.45639) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46192 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.55223) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79834 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.21581) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43531 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (0.57884) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50649 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.49234) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35974 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.34558) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73806 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.72390) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44768 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.43353) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85055 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.83640) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93190 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-1.91775) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73829 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.72414) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67086 HOMO: -7.09673 LUMO: 2.35106 factor:1 | -1 (1.34329) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68254 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (1.33162) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56198 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.45217) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10137 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.91278) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41093 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.60322) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35082 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.66333) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34545 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.33130) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41235 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.39820) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15385 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.13969) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98760 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.97345) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87126 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.85710) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00948 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.99533) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76456 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.75041) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06848 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.05433) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78826 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.77411) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50594 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.49179) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64441 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.63026) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68938 HOMO: -7.10761 LUMO: 2.20956 factor:1 | -1 (0.32477) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48650 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (0.52766) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43074 HOMO: -6.64502 LUMO: 1.38506 factor:1 | -1 (0.58341) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44173 HOMO: -6.87360 LUMO: 1.15648 factor:1 | -1 (0.57242) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54714 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.53299) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43106 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.41691) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22022 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.20607) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74624 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.73209) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28220 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.26805) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09044 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.07629) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94962 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.93546) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07398 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.05983) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91427 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.90012) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98914 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.97498) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06548 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-2.05133) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84845 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.83430) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70433 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.69018) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79429 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.78014) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12650 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.11235) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57604 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.56189) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50954 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.50461) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28076 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.26661) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48351 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.46936) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43110 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.41695) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44747 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.43331) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23166 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-2.21751) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46708 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.45292) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49222 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.47807) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89190 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.87775) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51829 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.50414) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42457 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.41042) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12791 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.11376) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17201 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.15785) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50438 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.49023) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58466 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.57051) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89204 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.87788) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20889 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.19474) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87528 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.86113) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13034 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-1.11618) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29725 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.28310) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33273 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-1.31858) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23134 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-2.21718) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99084 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.97669) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22423 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-2.21008) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13050 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-1.11635) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16040 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-1.14625) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86122 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.84706) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11395 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-2.09979) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14091 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-2.12676) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10910 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-2.09495) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22672 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-1.21257) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32922 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-1.31507) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93643 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.92228) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67196 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.65781) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05068 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-2.03653) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88752 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-1.87337) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32894 HOMO: -6.60420 LUMO: 2.20956 factor:1 | -1 (0.68521) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09726 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.08310) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95448 HOMO: -6.62597 LUMO: 1.70343 factor:1 | -1 (0.05967) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84199 HOMO: -6.69400 LUMO: 2.16875 factor:1 | -1 (1.17216) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37070 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.35655) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28915 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.27500) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20042 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.81373) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74241 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.72826) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96133 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.94717) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17401 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-1.15986) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83114 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-1.81699) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36998 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-2.35583) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36415 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-2.35000) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56417 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.55001) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19711 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-1.18296) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10464 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-2.09049) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21894 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.20479) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04879 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.03464) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89090 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.87675) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99281 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.97866) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94416 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-0.93000) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09110 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-1.07695) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09853 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-1.08437) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16029 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-2.14613) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37713 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-2.36298) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29270 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-2.27855) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36130 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-2.34715) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67614 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-1.66199) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47377 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-1.45962) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47237 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-2.45822) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11547 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-2.10132) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23819 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-2.22404) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25150 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-2.23735) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34902 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-2.33487) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28603 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-2.27188) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31085 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-2.29670) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31807 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-1.30392) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03682 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.02267) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09905 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.08490) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93735 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.92320) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07368 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.05953) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06783 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.05368) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00652 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-1.99236) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16315 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-1.14900) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19657 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-1.18242) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92918 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-1.91503) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05390 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.03975) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03003 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-2.01587) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50764 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.50651) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45239 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-0.43824) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68178 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-0.66763) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41772 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.40357) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43192 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.41777) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28204 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.26789) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53785 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-1.52370) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45642 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.44227) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72903 HOMO: -6.66951 LUMO: 1.68438 factor:1 | -1 (0.28512) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47712 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.46297) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72949 HOMO: -6.69128 LUMO: 2.13881 factor:1 | -1 (0.28466) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19266 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.17851) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56726 HOMO: -6.82189 LUMO: 2.46807 factor:1 | -1 (0.44689) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05746 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.04331) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17085 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-1.15670) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09893 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-1.08478) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36599 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-1.35183) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29652 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-1.28236) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30416 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.29001) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04416 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-1.03001) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85345 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-1.83930) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77906 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.76490) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68275 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-1.66860) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12045 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-2.10630) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87693 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-1.86278) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50027 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-1.48612) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98316 HOMO: -6.64230 LUMO: 2.11977 factor:1 | -1 (0.03099) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13731 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.12316) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14420 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.13004) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15515 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-1.14100) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97191 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.95776) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11937 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-1.10522) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86225 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-0.84810) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88271 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.86856) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19879 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-2.18464) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61239 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.59824) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30717 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-2.29302) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05484 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-2.04069) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14630 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-2.13215) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17558 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-2.16143) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43152 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.41737) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23097 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.21682) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26921 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (0.74494) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45016 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-0.43601) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36262 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.34847) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05661 HOMO: -6.87360 LUMO: 2.43270 factor:1 | -1 (0.95754) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66176 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.64760) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56622 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.55206) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21513 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.20097) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33227 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.31812) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64571 HOMO: -7.13483 LUMO: 1.47758 factor:1 | -1 (0.36844) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94871 HOMO: -6.72938 LUMO: 1.57282 factor:1 | -1 (0.06544) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25927 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.24512) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89849 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.88434) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84524 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.83109) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96010 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.94595) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86505 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.85090) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02990 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-1.01575) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91806 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.90391) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19279 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-1.17863) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55225 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-1.53810) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58618 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-1.57203) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65796 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-1.64381) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77291 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-1.75875) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20917 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.19502) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85683 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.84267) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80295 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.78879) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06257 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-2.04842) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31831 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.30416) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58275 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.56860) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23278 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-2.21863) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08297 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.06882) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36654 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.35239) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12097 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-1.10682) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00318 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.98903) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11627 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.10212) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20301 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (0.81114) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70033 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.68618) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40056 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-2.38641) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77840 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.76425) | 1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36531 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.35115) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04226 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.02811) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06985 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.05570) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38940 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.37525) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93324 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.91909) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92745 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.91330) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74333 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.72917) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11890 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-2.10475) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05028 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-1.03613) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86853 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.85438) | -1 | -1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07044 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-1.05629) | 1 | 1 |
| G: -5683.64846 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40169 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.38754) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01805 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.00390) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66249 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.64834) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16492 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.15077) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09406 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.07991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05243 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.03828) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03559 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.02143) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89550 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.88135) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83025 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.81610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11978 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.10563) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14076 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.12661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05159 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.03743) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84470 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.83055) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89959 HOMO: -7.26816 LUMO: 0.32926 factor:1 | -1 (0.11456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88492 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.87076) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66069 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.64654) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20615 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.19199) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06462 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.05047) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08299 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.06884) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31393 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.29978) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38348 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.36933) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42212 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.40797) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24199 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.22784) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75143 HOMO: -6.48992 LUMO: -0.25034 factor:1 | -1 (0.26273) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41374 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.39959) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62795 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.61380) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69119 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.67704) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82134 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.80719) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72012 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.70596) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91174 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-1.89759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96525 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.04890) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97241 HOMO: -6.55250 LUMO: 1.73064 factor:1 | -1 (0.04174) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77553 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.76137) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99648 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.98233) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90486 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.89071) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86935 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.85520) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94729 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.06686) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00187 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.98772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86824 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.85408) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64340 HOMO: -6.50896 LUMO: 1.73609 factor:1 | -1 (0.37076) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97801 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.96385) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30021 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-2.28606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14978 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-2.13563) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31749 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-2.30333) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.02038 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-3.00623) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.97780 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-2.96365) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27838 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-2.26423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78745 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-2.77330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.08858 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-3.07442) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41338 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-2.39923) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35218 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-2.33803) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32383 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.30968) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16724 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.15309) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13516 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.12101) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07651 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.06236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89678 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.88263) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03368 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.01953) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95918 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.94502) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86320 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.84905) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02582 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.01166) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85078 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.83663) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81759 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.80343) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94913 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.93497) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89888 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.88472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67476 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.66061) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82129 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.80714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55162 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.53747) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78292 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.76877) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83538 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.82123) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42514 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.41099) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75769 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.74354) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36941 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-2.35525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33969 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-2.32554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98698 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.97283) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95987 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.94572) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18333 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.16918) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16325 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-2.14910) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.07805 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-3.06389) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33126 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-2.31710) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10579 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.09164) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67334 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.65919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.46812 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-3.45397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.17108 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-3.15693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01696 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-2.00281) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99601 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.98186) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17895 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-2.16480) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51220 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.49805) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17672 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-2.16257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05786 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.04371) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42713 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.41298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60632 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.59217) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50655 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.49240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39354 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-2.37939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19759 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-2.18344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62076 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-2.60661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47187 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.45771) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19066 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.17651) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24095 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.22680) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19317 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.17901) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21839 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.20424) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01887 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-2.00472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07705 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-2.06290) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95448 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (0.05967) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26534 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.25119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98775 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.97360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29911 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.28496) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83671 HOMO: -6.87360 LUMO: 2.34290 factor:1 | -1 (0.17745) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62899 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.61484) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87455 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.86040) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68018 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.66603) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10666 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.09251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40180 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.38764) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86576 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.85161) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68651 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.67236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21656 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.20241) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15784 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-2.14369) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09008 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-2.07593) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99903 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.98488) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18442 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.82973) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93889 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.07527) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93965 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.07450) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87068 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.85653) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85805 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.84390) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79785 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.21630) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88759 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.12656) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73970 HOMO: -6.75659 LUMO: -0.45715 factor:1 | -1 (0.27445) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62788 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.61373) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65493 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.64077) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36931 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.35515) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52815 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.51400) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62580 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.61165) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73152 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.71736) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41722 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-2.40306) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18065 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.16650) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33890 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.32475) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38086 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-2.36671) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11401 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.09986) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54623 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.53208) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17703 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.16288) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81302 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.79887) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92657 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.91242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99930 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.98515) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12765 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.11350) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96021 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.94606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74755 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.73340) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73934 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.72518) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94799 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.93384) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79422 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.78007) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49731 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.48316) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67892 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (1.33524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45135 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.43720) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74056 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.72641) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63920 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.62505) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07188 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.05773) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70149 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-2.68734) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88224 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.86809) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42610 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.41194) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27283 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-2.25868) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61187 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.59772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49497 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.48082) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29185 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.27770) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32549 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.31134) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42358 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.40943) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47080 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.45665) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02594 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-2.01179) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13025 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-2.11609) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70231 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-2.68816) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13759 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.12344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43012 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.41597) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73930 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.72515) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69369 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.67954) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74382 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.72966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73276 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-2.71861) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78943 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.77528) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69838 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.68423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52183 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.50767) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89515 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.88100) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89869 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.88453) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84265 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.82850) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57500 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.56085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15053 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.13637) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12930 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.11515) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09634 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.08219) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13967 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.12552) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03901 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.02486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93400 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.91984) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74812 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.73397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63672 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.62257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89530 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (1.11885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77901 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.76486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86007 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.84592) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72102 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.70687) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81384 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.79969) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86941 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.85525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76168 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.74752) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80998 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.79582) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54823 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.53408) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93771 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.92355) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73438 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.72023) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65588 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.64173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83648 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.82233) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77852 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.76437) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85776 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.84361) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77817 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.76401) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91175 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.89759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64742 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.63326) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67952 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.66537) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76369 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.74954) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43195 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.41779) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54316 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.52901) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36933 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.35518) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29037 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.27621) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80821 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.79406) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80875 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.79460) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80198 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.78782) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62295 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.60880) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08303 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-2.06888) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77497 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.76082) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91425 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.90010) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68638 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.67223) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37871 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.36456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79568 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.78153) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90445 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.89030) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71735 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.70320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25898 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-2.24483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74556 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.73141) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37742 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.36326) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79304 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.77889) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21599 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-2.20184) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35388 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.33973) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68025 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.66610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82813 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.81397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91701 HOMO: -6.70216 LUMO: 1.93201 factor:1 | -1 (0.09714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24710 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.23295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37412 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.35997) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94026 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.92611) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00381 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (0.01034) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94602 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.93187) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99525 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.98110) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66638 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.65223) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50416 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-2.49001) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85936 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.84521) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14196 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.12781) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15830 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-2.14415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02761 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.01346) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09771 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.08356) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08691 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.07275) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02310 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.00894) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97977 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.96561) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57745 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.56330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70001 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.68586) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53785 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.52370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59579 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.58163) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66776 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.65361) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71780 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.70365) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77666 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.76251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10782 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-2.09367) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62180 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.60765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77281 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.75865) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82403 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.19013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85683 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.84268) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99406 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.97991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90228 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.88813) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00157 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.98742) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92353 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.90938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89430 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.88015) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73667 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.72252) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.37430 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.63985) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33326 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.31911) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25032 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.23617) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82883 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.81468) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55664 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.54249) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00802 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (2.00613) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.97956 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (2.03460) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85566 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.84151) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82111 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.80695) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19070 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.17655) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24760 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.23345) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25402 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.23987) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28850 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.27435) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86097 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.84682) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.68295 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (2.33120) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.74304 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (2.27112) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15776 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-2.14360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71601 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.70185) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40549 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-2.39134) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81624 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (0.19791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02459 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.01044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88699 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-2.87284) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33482 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-2.32067) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32785 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-2.31370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52906 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-2.51490) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83982 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.82567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89757 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.88342) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39810 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.38395) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03189 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.01774) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67563 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.66148) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05257 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.03842) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.31885 HOMO: -6.87360 LUMO: 1.15648 factor:1 | -1 (0.69531) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61013 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (1.40403) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42893 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.41478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10825 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.09410) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02814 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.01399) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57012 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.44404) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66429 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.65013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58878 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-2.57463) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25076 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-2.23661) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32108 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-2.30693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62066 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.60651) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91572 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.90157) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91994 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.90579) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88892 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.87476) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82089 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.80674) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63182 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.61767) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87286 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.85871) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16359 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.14944) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31227 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.29812) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.19779 HOMO: -6.90625 LUMO: 1.92384 factor:1 | -1 (1.81636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72182 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-2.70767) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06009 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-2.04594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39420 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.38005) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73775 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.72360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71705 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.70290) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77743 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.76328) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27028 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-2.25612) | 1 | 1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48525 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.47110) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80191 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.78776) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95697 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.94282) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17851 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.16436) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74927 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.73512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40961 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.39546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23616 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.22201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51568 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.50153) | -1 | -1 |