乙二醇作为反应物的反应表19-3

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: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52805 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.97857) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06945 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-2.51996) | 1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83420 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-3.28471) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24487 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-3.69539) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-2.68476) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17548 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-3.62600) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46156 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-2.91208) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86310 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-2.31362) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56981 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-3.02033) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83292 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-2.28344) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71476 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-3.16528) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96637 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-2.41689) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16330 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-2.61382) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29010 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-2.74062) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61077 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-2.06129) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93422 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-3.38474) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99883 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-2.44935) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07168 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-2.52220) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11581 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-2.56633) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-1.37208) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88586 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.33638) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99762 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-1.44814) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49267 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-2.94318) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67140 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-2.12192) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-1.99644) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85500 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.30552) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62950 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.08002) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83593 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.28645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64104 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.09156) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45273 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.90325) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49270 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-1.94322) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58546 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-2.03598) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79186 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-2.24238) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55531 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-2.00583) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11851 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-2.56903) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64916 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-3.09968) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91742 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-2.36793) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51729 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-2.96781) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80854 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-2.25906) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59177 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-3.04229) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-2.39613) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82370 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-2.27422) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94590 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-3.39642) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43783 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-2.88835) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54877 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-2.99929) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48132 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-2.93184) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08628 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-3.53680) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06531 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-2.51583) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20605 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-2.65657) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63809 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-2.08861) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43528 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.88580) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32308 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-2.77360) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19202 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-1.64253) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24617 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-1.69668) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53770 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-2.98822) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22293 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-1.67345) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23533 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-2.68585) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16564 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-2.61616) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70157 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-3.15209) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87978 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-2.33030) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30004 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-2.75055) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83361 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-2.28412) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35021 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-2.80073) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52009 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-2.97061) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76838 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-2.21890) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29233 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-2.74285) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49846 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-2.94898) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27277 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-2.72329) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13464 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-2.58516) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04751 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-2.49803) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92789 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-2.37841) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61254 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.06306) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17277 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-2.62329) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10449 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-2.55501) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26578 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-2.71629) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93731 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-2.38783) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36864 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-2.81915) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32970 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-2.78021) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19758 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-2.64810) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89891 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-2.34943) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00512 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-2.45564) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82694 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-2.27746) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55836 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-2.00888) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59083 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-2.04134) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95303 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-3.40355) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00272 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-2.45324) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29906 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-2.74957) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00466 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.45518) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99627 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-2.44679) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01852 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.46903) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96186 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.41238) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93759 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-1.38811) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11566 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.56618) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08208 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.53260) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19392 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.64444) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06780 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-1.51831) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00134 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-2.45185) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64519 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-2.09571) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95146 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-2.40198) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06331 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.51382) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28478 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-1.73530) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94080 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.39132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00856 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.45907) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94804 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.39856) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83119 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.28171) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30112 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-2.75164) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90673 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.35725) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88933 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-2.33985) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04617 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-3.49669) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41562 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-3.86614) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09200 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-3.54251) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60504 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-4.05556) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24283 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-3.69335) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48305 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-3.93357) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35066 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-1.80118) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.65410) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55765 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-2.00817) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79080 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-2.24132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09943 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-2.54995) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25669 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-2.70721) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93170 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-2.38222) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72492 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-2.17544) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-2.63749) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32218 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-3.77270) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41626 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-2.86677) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86078 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-3.31130) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07698 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-3.52749) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42560 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-1.87612) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33996 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-1.79048) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39813 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-2.84865) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50265 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-2.95317) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-2.86101) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87393 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-2.32445) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09211 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-2.54263) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26921 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-2.71972) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39223 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-2.84275) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03946 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-2.48998) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44279 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-2.89331) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08643 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-2.53694) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60595 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-2.05647) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50481 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.95533) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94147 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-2.39199) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31688 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-2.76740) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04262 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-2.49313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23541 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-2.68593) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00321 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-2.45373) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86555 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-2.31607) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35898 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.80950) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39326 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-2.84378) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79524 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-2.24576) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25672 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-2.70723) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22218 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-2.67270) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19141 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-2.64193) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35860 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.80912) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42045 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-2.87096) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40605 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-2.85657) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13005 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-2.58056) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55547 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-3.00599) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95361 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-2.40413) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-2.05100) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40132 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-2.85183) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34523 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-2.79575) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11913 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-2.56965) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-2.77994) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29217 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-2.74269) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46582 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.91633) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36666 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-1.81718) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42072 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-2.87124) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18882 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-2.63934) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26221 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-2.71273) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89932 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-2.34984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94106 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-2.39158) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64429 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-3.09481) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93931 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-3.38983) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78456 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-3.23508) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.28261 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-3.73313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90976 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-3.36028) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29409 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-3.74461) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47143 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-3.92195) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.78221 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-4.23273) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05172 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-3.50224) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22778 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-3.67830) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18998 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-3.64050) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52299 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.97351) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25413 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-2.70465) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19625 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-2.64677) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32295 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-2.77347) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27122 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-2.72174) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67419 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-3.12471) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04286 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-2.49338) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62450 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-3.07502) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20997 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-2.66048) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14798 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-2.59850) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20151 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-1.65203) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50639 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.95691) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18700 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-2.63752) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15125 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.60177) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12145 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-2.57197) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30069 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-2.75121) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60921 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-3.05973) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69344 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-2.14396) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08409 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-2.53460) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70356 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-2.15408) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58135 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-3.03187) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12656 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-2.57708) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23881 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-2.68933) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04087 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-2.49139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75678 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-3.20730) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-2.25786) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68148 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-3.13200) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28042 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-2.73093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26287 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.71339) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31119 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-2.76171) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.63650 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-4.08701) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.66539 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-4.11591) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70127 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-3.15179) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62490 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-4.07542) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51660 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-3.96712) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17960 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-2.63012) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09726 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-2.54777) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11894 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-2.56946) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88234 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-2.33286) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61286 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-3.06338) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95513 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-2.40565) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78525 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-2.23577) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82220 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-2.27272) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56197 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-3.01249) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15421 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-2.60473) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22012 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.67064) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20137 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-2.65189) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17451 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-2.62503) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26414 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-3.71465) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41661 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-2.86713) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-2.64818) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13243 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-3.58295) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09341 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-3.54393) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17383 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-2.62435) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90629 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-2.35681) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47010 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-3.92062) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22759 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-3.67811) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60578 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-3.05630) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10613 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-2.55665) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01255 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-2.46307) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18545 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-2.63597) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80411 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-2.25463) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13062 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-2.58114) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91570 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-2.36622) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06610 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-2.51662) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77009 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-2.22061) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71815 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-2.16867) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22624 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-2.67676) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18623 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-3.63675) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19002 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-2.64054) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90191 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-1.35243) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73285 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.18337) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13267 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-1.58319) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82746 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.27798) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00351 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-2.45403) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12243 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-2.57295) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85510 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-2.30562) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79520 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-3.24572) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04387 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-2.49439) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29040 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-2.74092) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36527 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.81579) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20287 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.65339) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47960 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-2.93012) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18611 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.63663) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19835 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-2.64887) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45154 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-3.90206) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07129 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-3.52181) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40614 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-1.85666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59768 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-2.04820) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59942 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-2.04994) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73379 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-2.18431) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-2.19849) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07887 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-1.52939) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-1.76520) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40525 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-3.85577) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99025 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-3.44077) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84932 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-3.29984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96656 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-2.41708) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95285 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-2.40336) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08240 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-2.53292) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85845 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-2.30897) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08180 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-2.53232) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98593 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-2.43645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17201 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-2.62252) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96768 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-2.41819) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99368 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-3.44420) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64084 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-2.09136) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92346 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-2.37398) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14275 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-2.59327) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13206 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-2.58258) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75181 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-2.20233) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65670 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-2.10722) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75736 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-2.20788) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44228 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-1.89280) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11376 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-1.56427) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30892 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-1.75943) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-1.28557) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.12338 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (0.42610) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26732 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-0.71784) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12269 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.57321) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23892 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-2.68944) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39130 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-2.84182) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96237 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-2.41289) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05121 HOMO: -6.92802 LUMO: -0.72927 factor:1 | -1 (0.49827) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96481 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.41533) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73298 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-2.18350) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29495 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-2.74547) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30617 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.75669) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90060 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-2.35112) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47683 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-2.92735) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56753 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-2.01805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16556 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-2.61608) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43262 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.88314) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09117 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-1.54169) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96494 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-1.41545) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67654 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-2.12706) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20908 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-1.65960) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22306 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.67358) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.32100) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05265 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.50317) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05218 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.50270) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89689 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.34741) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04030 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-2.49082) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21535 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-2.66587) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90406 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-2.35457) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26722 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-2.71774) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60438 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-2.05490) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36135 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-1.81187) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46875 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-2.91926) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43715 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-2.88767) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78737 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-2.23789) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45461 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-1.90512) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91004 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-2.36056) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13622 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-2.58674) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47477 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-1.92529) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20091 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-1.65143) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99151 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-2.44203) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21549 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-2.66601) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88778 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-2.33830) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60114 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-2.05166) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50423 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-2.95475) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13885 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-3.58937) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-2.88536) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74969 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-2.20020) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09100 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-2.54152) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89529 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-2.34581) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90729 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-2.35781) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11723 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-2.56775) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82898 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-2.27950) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59627 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-2.04679) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96691 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-2.41743) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69096 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-2.14148) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43586 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.88637) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05859 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-2.50911) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33354 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.78406) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17615 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.62667) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20874 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-2.65926) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17331 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-2.62383) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06956 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-2.52007) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00528 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-2.45580) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08355 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.53407) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13217 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-2.58269) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29002 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-2.74054) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77457 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.22509) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81681 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.26732) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73966 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.19018) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29337 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-2.74389) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21704 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-2.66756) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13306 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-3.58358) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53301 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-3.98353) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71504 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-3.16555) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74442 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-3.19494) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05462 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-1.50514) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91179 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.36231) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89487 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.34539) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97147 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-1.42199) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69238 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-2.14290) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69690 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-1.14742) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45415 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.90467) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70986 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-1.16038) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60209 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-2.05261) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93974 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-1.39026) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04305 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-2.49357) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93146 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-2.38198) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19673 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-3.64725) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25159 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-3.70211) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47675 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-2.92726) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05600 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-3.50651) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92585 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-2.37637) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15440 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-2.60492) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86065 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-2.31117) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82697 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-2.27748) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96082 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-2.41134) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71578 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-2.16630) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74573 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-3.19625) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78683 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-2.23735) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90819 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-2.35871) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72201 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-2.17253) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83921 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-2.28973) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71847 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-2.16899) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85605 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-2.30657) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97034 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-2.42086) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05476 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.50528) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76610 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.21662) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79592 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-2.24644) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56768 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.01820) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92736 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.37788) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87089 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.32141) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10922 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-3.55974) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27646 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-3.72698) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39647 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-2.84699) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88889 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-3.33941) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94335 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-2.39387) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04254 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-1.49306) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68166 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-2.13218) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69010 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.14062) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00921 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.45973) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92847 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-1.37899) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93187 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-2.38238) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12244 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.57295) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90783 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-3.35835) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07772 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-2.52824) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67888 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-2.12940) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96539 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-2.41591) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92892 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-3.37944) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99045 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-2.44097) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86667 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-2.31719) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75545 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-3.20596) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67447 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-2.12499) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01914 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.46966) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48151 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-2.93203) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92433 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-2.37485) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52992 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-2.98044) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51816 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-2.96868) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94838 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-2.39890) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37618 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.82670) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31389 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-2.76440) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23122 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-2.68174) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65406 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-2.10458) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13205 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.58257) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.20722 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (0.34226) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.22316 HOMO: -6.72665 LUMO: 2.12521 factor:1 | -1 (0.32632) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29914 HOMO: -6.67767 LUMO: 2.43814 factor:1 | -1 (0.25034) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67860 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.12912) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.94659 HOMO: -6.25046 LUMO: 1.77146 factor:1 | -1 (0.60290) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.02572 HOMO: -6.30488 LUMO: 1.90480 factor:1 | -1 (0.52376) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14808 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.59860) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21300 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.66352) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39450 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.84502) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26816 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.71868) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36370 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.81422) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04699 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.49751) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25701 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-2.70753) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96455 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-2.41506) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44635 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-2.89687) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-2.90389) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96335 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-2.41387) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62026 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-3.07078) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40172 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-2.85224) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68895 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-2.13947) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44227 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-2.89279) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41027 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-2.86079) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10983 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-2.56035) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79145 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-2.24197) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-2.39613) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08836 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-2.53888) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76688 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-2.21740) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35760 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.80811) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22936 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.67988) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55785 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-2.00836) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93061 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-2.38113) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94832 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.39884) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42597 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-2.87649) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53879 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-2.98931) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36958 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.82010) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49454 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-2.94506) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34736 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-2.79787) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-2.60116) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22073 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.67125) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33573 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.78625) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13665 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.58717) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01801 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.46853) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92909 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-2.37961) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06143 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.51195) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93228 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.38280) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25068 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.70120) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99094 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.44146) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17261 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.62313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80479 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-2.25531) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82989 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.28040) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44784 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.89836) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41959 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.87011) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00805 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.45857) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93354 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.38406) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35034 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.80086) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28030 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.73082) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89065 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.34117) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15414 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-1.60466) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17630 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.62681) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30713 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.75765) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.54654) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59963 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-3.05015) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55958 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-3.01010) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26534 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-2.71586) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26042 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-2.71093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53433 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-2.98484) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12108 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-3.57160) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01480 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-3.46532) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30327 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-2.75379) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58071 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-4.03123) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71520 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-3.16572) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45557 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-3.90609) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62595 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-3.07646) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12089 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-3.57141) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37762 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-2.82813) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55541 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-3.00593) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80328 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-3.25380) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07941 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-2.52992) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53141 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-2.98193) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31140 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-0.76192) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45377 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-0.90429) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64411 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-2.09462) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61651 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-2.06703) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30619 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.75671) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02047 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-2.47098) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.76520) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92964 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.38016) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02213 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-1.47265) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86915 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.31967) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16127 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.61178) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95778 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.40830) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16768 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-2.61820) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91094 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-2.36146) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11829 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-2.56881) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18912 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-2.63964) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73189 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-2.18241) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15613 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-3.60665) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45525 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-2.90577) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41585 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-2.86637) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19412 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-3.64464) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47027 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-2.92079) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17519 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-2.62571) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70619 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-3.15671) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82285 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-3.27337) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11225 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-2.56277) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79945 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-2.24997) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13816 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-2.58867) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02812 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.47864) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44533 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.89584) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50927 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.95979) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20286 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-2.65338) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40782 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-2.85834) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30080 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-2.75132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77199 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-3.22251) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19892 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-2.64944) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08455 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-2.53507) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32725 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-2.77777) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30599 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-2.75651) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08654 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.53706) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75114 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.20165) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.91380 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (0.63569) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.73709 HOMO: -6.25590 LUMO: 1.86670 factor:1 | -1 (0.81240) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05096 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.50148) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89426 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-2.34478) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39743 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-2.84794) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52810 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.97862) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14510 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.59562) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83773 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.28825) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84938 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.29990) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00029 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.45081) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03232 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.48284) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93365 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.38417) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17992 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-2.63044) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-2.62525) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07105 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-2.52157) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34657 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-2.79709) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68304 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-2.13356) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50203 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.95255) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42935 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.87987) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15614 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-2.60666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12093 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-2.57145) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42421 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-1.87473) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00964 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.46016) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23052 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.68104) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74264 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-2.19316) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28520 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.73571) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26057 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.71109) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28566 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.73618) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26922 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.71974) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24781 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.69833) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94788 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.39840) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23747 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.68799) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14846 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-0.59898) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01651 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.46703) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51710 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-2.96762) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37163 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-2.82215) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70106 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-2.15158) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33434 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.78486) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34398 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.79450) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59133 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-3.04185) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32568 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.77620) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33745 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-2.78797) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23620 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-2.68672) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22873 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.67925) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32424 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.77476) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77817 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-0.22868) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77632 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.22683) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10870 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.55922) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84336 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.29388) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03218 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.48270) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98078 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.43130) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04082 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-2.49134) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10325 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.55377) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12695 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.57747) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01614 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-2.46666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13985 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.59037) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83495 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.28547) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79589 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-2.24641) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01647 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.46699) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99682 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-2.44734) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23686 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.68738) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99005 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-1.44057) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37114 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-2.82166) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49120 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-2.94171) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19742 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-2.64794) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13241 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-2.58293) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24104 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-2.69156) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11433 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.56485) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99100 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-2.44151) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-2.76762) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41432 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-2.86484) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78170 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.23222) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29287 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.74339) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88127 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.33179) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61446 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.06498) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21808 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-1.66860) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96970 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-1.42022) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05628 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.50680) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05032 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-2.50084) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12039 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-1.57091) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67894 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-2.12945) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76166 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-2.21218) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78452 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.23504) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03495 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.48547) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96207 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-2.41259) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10377 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-1.55429) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22987 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.68039) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08002 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.53054) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05469 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.50521) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90470 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.35522) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.64758 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.09810) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27477 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.72529) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37701 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.82753) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86753 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.31805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.14975 HOMO: -6.80013 LUMO: 2.12249 factor:1 | -1 (0.39974) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48871 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.93923) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36201 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.81253) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98973 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.44025) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93664 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.38715) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15039 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.60091) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.77433) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22547 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.67599) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34517 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.79569) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37837 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.82889) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52743 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.97795) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.42201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15378 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.60430) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84610 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.29662) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25457 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.70509) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95887 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.40939) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30310 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.75362) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27790 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.72842) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97364 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.42416) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92904 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-1.37956) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25898 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.70950) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91391 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.36443) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63083 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-1.08135) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00820 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.45872) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40691 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.85743) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32838 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.77890) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20593 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.65645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35733 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.80785) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05678 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.50730) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31091 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.76143) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24103 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.69155) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87025 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.32077) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12326 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.57378) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70961 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.16013) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45182 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-2.90234) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44951 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-2.90003) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36298 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-2.81349) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56140 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-3.01192) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31182 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-2.76234) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24934 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-2.69986) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43468 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-2.88520) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01731 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-2.46783) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02351 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-2.47403) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48692 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-2.93744) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99589 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-2.44641) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45705 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-2.90756) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71385 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-2.16437) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22229 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-2.67281) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32809 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-2.77861) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35272 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-2.80324) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38994 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-2.84046) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53755 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.98806) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43038 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-2.88090) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-2.57610) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.42201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78037 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.23089) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31753 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-2.76805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20474 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-2.65526) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94087 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-2.39139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44445 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-2.89496) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50320 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-2.95371) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11408 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-1.56460) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27435 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-2.72487) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01315 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-2.46366) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67087 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.12139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.72987 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.18038) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.53827 HOMO: -6.68584 LUMO: -0.69389 factor:1 | -1 (0.01121) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04149 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.49201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88181 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.33233) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98027 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-2.43079) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98447 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.43499) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79089 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.24141) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91518 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-2.36570) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01816 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-1.46868) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66499 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-1.11550) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66623 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-2.11675) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71750 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.16802) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42743 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.87795) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85928 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.30980) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19028 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.64080) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97352 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.42404) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90845 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.35897) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10263 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.55315) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15379 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.60431) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31194 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.76246) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68087 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-2.13139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39354 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.84406) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91663 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-2.36715) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00008 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-2.45060) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00077 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-1.45129) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01283 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-1.46335) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06585 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-3.51636) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37936 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-2.82988) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02944 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-3.47996) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25503 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-2.70555) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39333 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-3.84385) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12232 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-2.57284) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64478 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-3.09530) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75346 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-3.20398) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06194 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-2.51245) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79706 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-2.24758) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71747 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-2.16799) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61591 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-2.06643) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84937 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-1.29989) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.26923 HOMO: -6.76747 LUMO: -0.67484 factor:1 | -1 (0.28025) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.96710 HOMO: -7.23279 LUMO: 0.48980 factor:1 | -1 (0.58238) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01897 HOMO: -6.62869 LUMO: -0.24762 factor:1 | -1 (0.53051) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89972 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.35024) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88905 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.33957) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70486 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-0.15538) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77242 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.22294) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.65275 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.10327) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95175 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.40227) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04530 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.49582) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92524 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.37576) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16481 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.61533) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65252 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.10304) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70279 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.15331) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.75961 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.21013) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67729 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.12781) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.33416 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (0.21532) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40662 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (0.14286) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43777 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.88829) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.03478 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (0.51470) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.31990 HOMO: -6.81917 LUMO: 2.41365 factor:1 | -1 (0.22958) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01309 HOMO: -6.40284 LUMO: 2.48984 factor:1 | -1 (0.53639) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.06150 HOMO: -7.04775 LUMO: 2.31025 factor:1 | -1 (0.48798) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.80016 HOMO: -6.64774 LUMO: 2.20140 factor:1 | -1 (0.74932) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.86735 HOMO: -6.72393 LUMO: 2.28304 factor:1 | -1 (0.68214) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.85516 HOMO: -6.35114 LUMO: 1.84765 factor:1 | -1 (0.69433) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38182 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.83234) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26658 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.71710) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24261 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.69313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44025 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.89076) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19684 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.64736) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07523 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.52575) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.61879) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96650 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.41701) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74962 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.20014) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73392 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.18444) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.43971 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (0.10977) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84878 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-0.29930) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88611 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.33663) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75073 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.20125) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43265 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.88317) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89397 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-1.34449) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88548 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.33600) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84210 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.29262) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20570 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-1.65622) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64343 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.09395) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49666 HOMO: -6.94707 LUMO: 1.81500 factor:1 | -1 (0.05282) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.39887 HOMO: -6.39468 LUMO: 1.79051 factor:1 | -1 (0.15062) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03648 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.48700) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15679 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.60730) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43635 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.88687) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52548 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-2.97600) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29761 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.74813) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02011 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-2.47063) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08825 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-2.53877) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39873 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-2.84925) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82871 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-2.27923) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51699 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-2.96751) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96196 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-2.41248) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55297 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-3.00348) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32850 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-2.77902) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75031 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-2.20083) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37098 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-2.82149) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10224 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-2.55275) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81483 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-2.26535) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52693 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-1.97745) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28066 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-2.73118) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33770 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-2.78821) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43088 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.88140) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35941 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-2.80993) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00525 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-3.45576) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96418 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-3.41470) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32714 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-2.77766) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08693 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-3.53745) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51486 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-3.96538) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41680 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-2.86732) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71754 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-3.16806) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53263 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-3.98315) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10830 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-2.55882) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-2.62525) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85550 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-3.30602) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46603 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-2.91654) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68269 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-2.13321) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61436 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-2.06488) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66895 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-2.11947) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50654 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-2.95706) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25142 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.70194) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45675 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-2.90726) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51364 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-2.96416) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13080 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-3.58132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40047 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-2.85099) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11896 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-3.56948) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47748 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-2.92800) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18351 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-3.63403) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.46452 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-3.91504) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64412 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-3.09464) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07777 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-2.52829) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93493 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-3.38545) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45544 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-2.90596) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76845 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-3.21897) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34209 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.79261) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14998 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.60050) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27535 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.72586) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04841 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-2.49893) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-1.55739) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78099 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-1.23151) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78872 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.23923) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06184 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-1.51235) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82300 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-1.27352) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92940 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-1.37992) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67475 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-1.12527) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03318 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-1.48370) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61367 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-3.06419) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24468 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-3.69520) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64848 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-3.09900) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51290 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-3.96342) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06775 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-3.51827) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86095 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-2.31147) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79950 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-3.25002) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83267 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-3.28319) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18322 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-2.63374) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54146 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.99198) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-2.71681) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12188 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-2.57240) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39895 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-2.84947) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52001 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-2.97053) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90072 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-1.35124) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10628 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.55680) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19304 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-2.64356) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94844 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-2.39896) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31106 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-2.76157) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.68772 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.13823) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30307 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.75359) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89962 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-2.35014) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23607 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.68659) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12532 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.57584) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79687 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-2.24739) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61635 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-2.06687) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37547 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-2.82598) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04887 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-2.49939) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64721 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-2.09773) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83146 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-2.28197) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01462 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-1.46514) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71372 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.16424) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99007 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-2.44059) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15313 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.60365) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91930 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.36982) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46018 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-1.91070) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00413 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.45465) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24869 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-2.69921) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57152 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-3.02204) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53686 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-2.98737) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60246 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-3.05298) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30465 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-0.75517) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15445 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-2.60497) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27216 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-0.72268) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32196 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-0.77248) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96241 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-0.41293) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22947 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.67999) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03894 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-2.48946) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09729 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.54781) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16352 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.61404) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73205 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-2.18257) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89405 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.34457) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30859 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.75911) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39118 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.84169) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10927 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.55978) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12770 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.57821) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36756 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.81808) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30612 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.75664) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43853 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-0.88905) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84012 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.29064) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40884 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.85935) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88765 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-2.33817) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79105 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-2.24157) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16259 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-2.61311) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45735 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.90787) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97929 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-2.42981) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28172 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-2.73224) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29267 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-1.74319) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83728 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-2.28780) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19108 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-2.64160) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83099 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-2.28151) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12200 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-1.57252) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86366 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-1.31417) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28051 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.73103) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99672 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-1.44724) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72675 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-2.17726) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39093 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.84145) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18149 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.63201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20253 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.65305) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29875 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.74927) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17221 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.62273) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22664 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.67716) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87526 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.32577) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88903 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-0.33954) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13600 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.58651) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73778 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.18830) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12683 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.57734) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04203 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.49255) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46984 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-1.92036) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95253 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.40305) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09331 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-2.54383) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70483 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-3.15535) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32668 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-2.77719) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40902 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-2.85954) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14711 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-2.59763) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96074 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-2.41126) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93230 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-2.38282) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12300 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-2.57352) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15949 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-2.61001) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74698 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.19750) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11374 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.56426) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89542 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.34594) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94317 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.39369) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57146 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.02198) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69875 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-2.14926) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04055 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-2.49107) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10399 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.55450) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37006 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-1.82058) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64827 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-2.09879) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81274 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-1.26326) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66275 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.11327) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80773 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-2.25825) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-1.37208) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76295 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.21346) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10423 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.55475) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98827 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-0.43878) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50585 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.95637) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35295 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23926 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.68978) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85400 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.30452) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04895 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.49946) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07540 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.52591) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12315 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.57367) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32751 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.77803) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25374 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.70426) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28196 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.73248) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96933 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.41984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01798 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.46850) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61593 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.06645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86053 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.31105) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37486 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-0.82538) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33045 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.78097) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20933 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.65985) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36833 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.81885) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88965 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.34017) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88761 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.33813) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22250 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-0.67302) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04984 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.50036) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79949 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-1.25001) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64286 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-1.09338) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85389 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-1.30441) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64202 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.09254) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29847 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.74899) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33431 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.78483) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44295 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-2.89347) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44409 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-2.89461) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41664 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-2.86715) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17894 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-2.62946) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13870 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-2.58922) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19704 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-2.64756) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23413 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-2.68465) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09312 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-2.54364) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14120 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-2.59172) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15372 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-2.60424) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01472 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-2.46524) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95388 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-2.40440) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16817 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-2.61869) | -1 | -1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84536 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-2.29588) | 1 | 1 |
| G: -5715.18379 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02536 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-2.47588) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95534 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-3.40586) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19416 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-2.64467) | 1 | 1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01357 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-3.46409) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-2.76860) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85115 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-3.30167) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34923 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-3.79974) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-2.63749) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97077 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-3.42129) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81890 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-3.26942) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09617 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-2.54669) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89071 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-3.34123) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27739 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-3.72791) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06909 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-2.51961) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25048 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-2.70100) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63795 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-3.08847) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92542 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-2.37593) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75691 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-3.20743) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13312 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-2.58364) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18501 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-2.63553) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95246 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-3.40297) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21522 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-2.66574) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00406 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-2.45458) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20422 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-2.65474) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11782 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-3.56834) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11447 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-3.56499) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71066 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-3.16117) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82601 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.27653) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27710 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-2.72761) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12118 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-2.57169) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23870 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-2.68922) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29462 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.74514) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91929 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-2.36981) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43465 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-2.88517) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62336 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-3.07388) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41106 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-2.86158) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-2.79616) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24931 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-2.69983) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06273 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.51325) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30011 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-0.75063) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00437 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.45489) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92628 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.37680) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38899 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-2.83951) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32752 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-2.77804) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34643 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-2.79695) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23669 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-2.68721) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-2.76860) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27424 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-2.72476) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24341 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-2.69393) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12183 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-2.57235) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18048 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-1.63100) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24627 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-2.69678) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14206 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.59258) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89635 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.34686) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07017 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.52069) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93866 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.38918) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02765 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-2.47817) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17846 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-1.62898) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88332 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-2.33384) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92929 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.37981) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93314 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-2.38366) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13868 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.58920) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10633 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.55685) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15327 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.60378) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93362 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-1.38413) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94083 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.39135) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87751 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.32802) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62928 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.07980) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72455 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.17507) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06197 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-1.51249) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94736 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-1.39788) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31001 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.76053) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88725 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.33777) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62879 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-1.07931) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.51587 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.96639) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94646 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.39698) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67459 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-1.12511) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38153 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-2.83205) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34766 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-2.79817) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14534 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-2.59586) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83075 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-2.28127) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91597 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-2.36649) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75777 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-2.20829) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43705 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.88757) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64043 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-2.09095) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31644 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-2.76696) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43902 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-3.88954) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42134 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-2.87186) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.36065 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-3.81117) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71036 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-3.16087) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06795 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-2.51847) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81270 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-3.26322) | 1 | 1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40431 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-2.85483) | 1 | 1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48466 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-2.93518) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27701 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-2.72753) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79275 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-3.24327) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98422 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-2.43474) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89396 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-2.34448) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29993 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-2.75045) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05619 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-3.50670) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94277 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-3.39329) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13288 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-2.58339) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05783 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-2.50835) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40428 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-2.85480) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52498 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.97550) | 1 | 1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91215 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.36266) | 1 | 1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67048 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.12100) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80189 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-1.25240) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17753 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-2.62805) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29819 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-2.74870) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89869 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-2.34921) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65743 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-3.10795) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54678 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.99730) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62392 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-1.07444) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55810 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-1.00862) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47407 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.92459) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77650 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-1.22702) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93968 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.39020) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66654 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.11705) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89535 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-2.34587) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99301 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-2.44353) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71330 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-2.16382) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47012 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-1.92063) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81875 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-2.26927) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62794 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-2.07846) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12749 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-2.57801) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62929 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-3.07981) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87950 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-3.33002) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04044 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-2.49096) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19973 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-3.65024) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69615 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-3.14667) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48330 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-2.93382) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70192 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-3.15244) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92218 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-2.37270) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80871 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-2.25923) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11733 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-3.56785) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30499 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-2.75551) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16795 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-2.61847) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16705 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-2.61757) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82865 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-2.27917) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83575 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-2.28627) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75709 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-2.20761) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66457 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-2.11509) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23963 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-2.69014) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33538 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-2.78590) | -1 | -1 |
| G: -5715.18379 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72185 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-2.17237) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58653 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-2.03704) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24578 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-1.69630) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30999 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-2.76051) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23432 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-2.68484) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04966 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-2.50018) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81448 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-2.26499) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92104 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-2.37155) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11881 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-2.56933) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81647 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.26699) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82593 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-2.27645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87268 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-2.32320) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08328 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.53380) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87487 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.32538) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93530 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.38582) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06711 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.51763) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11185 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-1.56237) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13852 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-1.58904) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89476 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-1.34528) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53935 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.98987) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18584 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.63636) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04333 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.49385) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58759 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-2.03811) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08218 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-2.53270) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95033 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-3.40085) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91867 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-2.36919) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91339 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-2.36391) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04755 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-1.49807) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82866 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-1.27918) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84061 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.29113) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79642 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.24693) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98058 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-1.43110) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83726 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-1.28778) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93446 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-1.38498) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79791 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-1.24843) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09565 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-2.54617) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24893 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-2.69945) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82480 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.27532) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85176 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.30228) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-2.25786) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86041 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-2.31093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38572 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-2.83624) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43532 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-3.88584) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51614 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-3.96666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69196 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-3.14248) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50896 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-3.95947) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23997 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-3.69049) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42613 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-2.87665) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43997 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.89048) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39789 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-2.84841) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42885 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-2.87937) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46886 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.91938) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55646 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-2.00698) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28031 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-2.73083) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24093 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-2.69145) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13765 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.58817) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71926 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-2.16978) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36701 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.81753) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45394 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-2.90446) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23873 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-2.68925) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41330 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.86382) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51681 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.96733) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90544 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-2.35596) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12256 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-2.57308) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30967 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-2.76019) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13261 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-1.58313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75584 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.20636) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07593 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.52645) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35063 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.80115) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26316 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-2.71368) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12738 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-2.57790) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51572 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.96624) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32255 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.77307) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13239 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-2.58290) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61596 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-3.06648) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70013 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-2.15065) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06901 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-2.51953) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29916 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-3.74967) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61767 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-4.06818) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.76131 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-4.21183) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19496 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-3.64548) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.57807 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-4.02859) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78505 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-3.23557) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20216 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-2.65267) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64023 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-3.09075) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43518 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.88569) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60669 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-2.05721) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04060 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-2.49112) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76773 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-2.21824) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63653 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-3.08705) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84411 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-2.29463) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91277 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-1.36329) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84066 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.29118) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70384 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-1.15436) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92022 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-2.37074) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27278 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.72330) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23365 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.68417) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04918 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.49970) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05527 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-2.50579) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95442 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-3.40493) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25574 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-2.70625) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32465 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-3.77517) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-2.67578) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11137 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-3.56189) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18432 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-3.63484) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41816 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-2.86868) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44475 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-2.89526) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06760 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-1.51812) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97875 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-2.42927) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93067 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-2.38119) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87943 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-2.32995) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06319 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-2.51371) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97415 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-2.42467) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96030 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-2.41082) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93973 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-2.39025) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94251 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-2.39302) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87385 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-2.32437) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15794 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-2.60846) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90748 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-2.35800) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70090 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-2.15141) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74830 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-2.19882) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43980 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.89032) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70606 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-3.15658) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97647 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-2.42698) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85107 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-2.30159) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99660 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-2.44712) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98106 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-2.43158) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70753 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-2.15805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82833 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-2.27884) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69235 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-2.14287) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50174 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.95225) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95377 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-2.40429) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07840 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-2.52892) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10896 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-2.55948) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23543 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-3.68595) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17415 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-3.62467) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35669 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-2.80721) | 1 | 1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91734 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-1.36786) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65244 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-1.10296) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48327 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.93379) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80262 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.25314) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73405 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.18457) | -1 | -1 |
| G: -5715.18379 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62318 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-2.07370) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99320 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-2.44372) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75717 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-2.20769) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52677 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.97729) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68903 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-2.13955) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87611 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-2.32663) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94435 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-3.39487) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99198 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-2.44249) | 1 | 1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73542 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-3.18594) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80482 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-2.25533) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50067 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.95119) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67616 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-2.12668) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43022 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.88074) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89235 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-2.34287) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83535 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-2.28587) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33887 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-2.78938) | 1 | 1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62927 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-2.07979) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22188 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-2.67240) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49597 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.94648) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23476 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.68528) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33569 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.78621) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96885 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.41937) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94786 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.39837) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84859 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.29911) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07970 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.53021) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94073 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-0.39125) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12681 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-2.57733) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34235 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-2.79287) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93399 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-2.38451) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27051 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-2.72103) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60753 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-2.05805) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48206 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-1.93258) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40026 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-2.85077) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42635 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-2.87687) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76890 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-2.21942) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19391 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.64443) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23840 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-2.68892) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58457 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-2.03509) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04667 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-2.49719) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37286 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.82338) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22900 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-1.67951) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02003 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-2.47055) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89954 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-2.35006) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47822 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.92874) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41609 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-2.86661) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-2.79616) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28912 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-2.73964) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32300 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.77352) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15323 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-2.60375) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.65410) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21916 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-2.66968) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43664 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-2.88716) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88786 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.33837) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87643 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.32694) | -1 | -1 |
| G: -5715.18379 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94127 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.39179) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06097 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.51149) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33507 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.78558) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92420 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.37472) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66986 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.12037) | 1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04347 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.49399) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70596 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-2.15648) | -1 | -1 |
| G: -5715.18379 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85615 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.30666) | 1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87484 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.32536) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86171 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-2.31223) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05041 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.50093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94417 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.39469) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94894 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.39945) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.41781 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.13168) | -1 | -1 |
| G: -5715.18379 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08514 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.53566) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31053 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.76105) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92854 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.37905) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03148 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.48200) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13034 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.58085) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29292 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.74344) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71666 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.16718) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94420 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.39472) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89025 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.34077) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88315 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-0.33367) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87594 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.32645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09684 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.54736) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10400 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.55451) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34817 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-2.79869) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97429 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-2.42481) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41294 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-2.86345) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31010 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-2.76062) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04490 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-2.49542) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27663 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-2.72715) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05464 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-2.50516) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76247 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-2.21299) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17280 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-2.62331) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83427 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.28479) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46149 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.91201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77696 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.22748) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21531 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.66583) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56349 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.01401) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38219 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-2.83271) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33944 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-2.78996) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74770 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-2.19822) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-2.71681) | -1 | -1 |
| G: -5715.18379 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26284 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-2.71336) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67806 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.12858) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26758 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.71810) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04477 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.49528) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44639 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.89691) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99081 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.44133) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69686 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.14738) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.91626 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.36678) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98176 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.43228) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.04270 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.50678) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29195 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.25753) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.25568 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.29380) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05821 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.49127) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12024 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.57076) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74597 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.19649) | 1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93409 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.38461) | 1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99978 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.45029) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14574 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.59626) | 1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76540 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.21592) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65981 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.11033) | 1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09228 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.54280) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81630 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.26682) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30039 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.75091) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74011 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.19063) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37166 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.82218) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37171 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.82223) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81241 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.26293) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49686 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.94737) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25590 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.70642) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.57289) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12550 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.57602) | -1 | -1 |
| G: -5715.18379 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47028 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.92080) | 1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35552 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.80604) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51980 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.97032) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31470 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.76522) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.59012) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25952 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.71004) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99701 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.44753) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28908 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.73960) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56536 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.01587) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29365 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.74417) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83423 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.28475) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66106 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.11158) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83026 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.28078) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95764 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.40816) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08619 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.53671) | 1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31485 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.76537) | 1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11980 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.57031) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81297 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.26349) | 1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05017 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.50069) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90116 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.35168) | 1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21953 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.67004) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36513 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.81565) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85317 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.30369) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37674 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.82726) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36627 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.81679) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08398 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.53450) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15870 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.60922) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10743 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.55795) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41782 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.86833) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14426 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.59478) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29794 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.74846) | -1 | -1 |
| G: -5715.18379 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87619 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.32671) | 1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77876 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.22928) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84769 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.29821) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04160 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.49212) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12076 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.57128) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88391 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.33443) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80533 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.25585) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82126 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.27178) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60364 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.05416) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74945 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.19997) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55045 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.00097) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80515 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.25567) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82163 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.27215) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95158 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.40209) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74790 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.19842) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05743 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.50795) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85451 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.30503) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97284 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.42335) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97926 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.42978) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77906 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.22957) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80622 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.25674) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02818 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.47870) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07531 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.52583) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84742 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.29794) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39598 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.84650) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59433 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-3.04485) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.61515) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07688 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.52739) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29737 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.74789) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82128 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.27180) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48784 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-3.93836) | -1 | -1 |
| G: -5715.18379 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59914 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-3.04966) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40172 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-3.85223) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39936 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.84988) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57844 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-3.02895) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91665 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-3.36716) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19620 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.64672) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90275 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.35327) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11451 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.56503) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83313 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-3.28365) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76674 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-3.21726) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04716 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.49768) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32991 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.78043) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98965 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-3.44017) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91452 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-3.36504) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20480 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.65531) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82531 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.27582) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34956 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.80008) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09532 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.54584) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88592 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.33644) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.54654) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32856 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.77908) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43958 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.89010) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15416 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.60468) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97988 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.43039) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69989 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.15041) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85641 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.30693) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00801 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.45853) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89966 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.35017) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61938 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.06990) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84072 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.29123) | -1 | -1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18703 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.63755) | 1 | 1 |
| G: -5715.18379 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85184 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.30236) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79309 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.24361) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70988 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.16039) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02520 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.47572) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86433 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.31485) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30485 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.75537) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32193 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-3.77245) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71308 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-3.16360) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86132 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-3.31184) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15908 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.60960) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88705 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.33757) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69844 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-3.14896) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94068 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.39120) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92539 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.37591) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97012 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-3.42063) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24278 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.69330) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97368 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-3.42420) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72792 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.17843) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97192 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.42244) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81101 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-3.26153) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97627 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.42679) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.19849) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60985 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.06036) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53406 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.98458) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07345 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.52396) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22994 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.68046) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98874 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.43926) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14565 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.59617) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98023 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.43075) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01872 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-3.46923) | -1 | -1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25799 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.70851) | 1 | 1 |
| G: -5715.18379 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90853 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.35905) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97588 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-1.42639) | 1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85986 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-2.31038) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98838 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.43890) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51666 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-3.96718) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50969 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-3.96021) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17258 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-2.62310) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16273 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-2.61325) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16428 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.61480) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23139 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.68191) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36679 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.81731) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22146 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-1.67198) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39406 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.84458) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41776 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.86828) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57662 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-2.02714) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25767 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-2.70819) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.44746 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-3.89798) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03406 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-3.48458) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16117 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-3.61169) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14041 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-2.59093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79733 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-2.24785) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98618 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-2.43670) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96272 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-2.41324) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76585 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-2.21637) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97045 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.42097) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01600 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-2.46652) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80667 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-2.25718) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99938 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-2.44990) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04783 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-3.49835) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82914 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-2.27966) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84985 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.30037) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82781 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-2.27833) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85630 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-2.30682) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54563 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.99615) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66261 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-2.11313) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74539 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-2.19590) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44394 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.89446) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94528 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-2.39580) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04194 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.49246) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01250 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.46302) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12399 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.57451) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.17334 HOMO: -6.88176 LUMO: 0.71566 factor:1 | -1 (0.37614) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98324 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-2.43376) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03013 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-2.48064) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-2.65183) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58005 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-2.03057) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26208 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.71259) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50399 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.95451) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08224 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-2.53275) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00407 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.45458) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71992 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-2.17043) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29503 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-2.74555) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16967 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.62019) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23955 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.69007) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99598 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.44650) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18159 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.63211) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87590 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.32642) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55056 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.00108) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38981 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-1.84033) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07960 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.53012) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81103 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.26155) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86881 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.31933) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87071 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.32123) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22817 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-2.67869) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89301 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-2.34353) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83970 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-2.29022) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03889 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-2.48941) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10194 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-2.55246) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11206 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.56258) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45403 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.90455) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12479 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-2.57531) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46160 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.91212) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27468 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-1.72520) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03679 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-2.48731) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37207 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.82259) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15014 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.60066) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05894 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-2.50946) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24344 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-2.69395) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57880 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-2.02932) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35806 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-1.80858) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21478 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-2.66530) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88566 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-2.33618) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78158 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-2.23210) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96996 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-2.42048) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21631 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-1.66683) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40078 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-1.85130) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03566 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.48618) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48575 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-2.93627) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97004 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-2.42056) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82587 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-3.27639) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32110 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-2.77162) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89157 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-2.34208) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78269 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-2.23321) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78087 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-2.23139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82299 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-2.27351) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69216 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-2.14268) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46718 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-1.91770) | 1 | 1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89323 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-2.34374) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52603 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.97655) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36228 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.81280) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58160 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-2.03212) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59118 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-2.04170) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79992 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-2.25044) | -1 | -1 |
| G: -5715.18379 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87731 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-2.32783) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16644 HOMO: -6.70489 LUMO: -0.52518 factor:1 | -1 (0.28254) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55948 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.11051) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40174 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (1.04723) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48163 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.96734) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37668 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (1.07229) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45962 HOMO: -6.24501 LUMO: -0.44627 factor:1 | -1 (0.98935) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50193 HOMO: -6.73754 LUMO: -0.45443 factor:1 | -1 (0.94704) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43216 HOMO: -6.24501 LUMO: 0.38096 factor:1 | -1 (1.01681) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47709 HOMO: -6.86815 LUMO: -0.91974 factor:1 | -1 (0.97188) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06097 HOMO: -7.40150 LUMO: 0.36191 factor:1 | -1 (0.38801) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17759 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.27138) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19719 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (0.25179) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-0.09695) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46677 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.01780) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26871 HOMO: -7.34163 LUMO: 0.30477 factor:1 | -1 (1.18027) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40876 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (1.04021) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11442 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (1.33456) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38253 HOMO: -6.75659 LUMO: -0.68845 factor:1 | -1 (1.06644) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39693 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (1.05205) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17667 HOMO: -6.28583 LUMO: -0.46804 factor:1 | -1 (0.27230) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87269 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (0.57628) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06785 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.38112) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19310 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.25587) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38095 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (1.06802) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44988 HOMO: -6.36202 LUMO: -0.14422 factor:1 | -1 (0.99909) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14434 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.30463) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06932 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.37965) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14551 HOMO: -6.84638 LUMO: 1.88575 factor:1 | -1 (0.30346) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44173 HOMO: -5.90759 LUMO: 2.00820 factor:1 | -1 (0.00724) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37505 HOMO: -6.56339 LUMO: 1.99732 factor:1 | -1 (1.07392) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12941 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (1.31956) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35845 HOMO: -6.16882 LUMO: 1.94017 factor:1 | -1 (1.09052) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33594 HOMO: -6.80829 LUMO: 1.78507 factor:1 | -1 (1.11303) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39290 HOMO: -6.58243 LUMO: 1.78235 factor:1 | -1 (1.05607) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45965 HOMO: -5.85045 LUMO: 1.82316 factor:1 | -1 (0.98932) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32109 HOMO: -5.93752 LUMO: 1.56465 factor:1 | -1 (1.12788) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38065 HOMO: -6.59604 LUMO: -0.53334 factor:1 | -1 (1.06832) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42474 HOMO: -7.06135 LUMO: 0.29660 factor:1 | -1 (1.02424) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07931 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (0.36967) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.68040 LUMO: -0.60681 factor:1 | -1 (0.57849) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18203 HOMO: -6.93618 LUMO: -1.09662 factor:1 | -1 (0.26694) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18187 HOMO: -6.72121 LUMO: -1.14016 factor:1 | -1 (1.26710) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32876 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (1.12021) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05128 HOMO: -6.71305 LUMO: -0.71566 factor:1 | -1 (0.39769) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06167 HOMO: -7.09401 LUMO: -0.86532 factor:1 | -1 (0.38730) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10853 HOMO: -7.08584 LUMO: -0.92519 factor:1 | -1 (0.34044) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10497 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.34401) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23483 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (1.21414) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06778 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (1.38120) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17567 HOMO: -6.81373 LUMO: -1.72248 factor:1 | -1 (1.27330) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99120 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (1.45777) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15401 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (1.29496) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12820 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (0.32077) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10271 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (0.34626) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34707 HOMO: -7.04231 LUMO: -0.83539 factor:1 | -1 (1.10190) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26558 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (1.18340) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40797 HOMO: -6.89809 LUMO: -1.19186 factor:1 | -1 (1.04100) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08408 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (1.36490) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12753 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (1.32144) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07131 HOMO: -6.84366 LUMO: -0.88437 factor:1 | -1 (1.37766) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21692 HOMO: -6.91986 LUMO: -1.12655 factor:1 | -1 (1.23205) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15626 HOMO: -6.49536 LUMO: -0.29660 factor:1 | -1 (0.29271) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27581 HOMO: -6.74842 LUMO: 0.42450 factor:1 | -1 (1.17316) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23864 HOMO: -7.34435 LUMO: 0.32109 factor:1 | -1 (1.21034) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03199 HOMO: -7.16476 LUMO: 0.28572 factor:1 | -1 (1.41698) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34248 HOMO: -6.74298 LUMO: -0.43538 factor:1 | -1 (1.10650) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34841 HOMO: -7.19469 LUMO: -1.61091 factor:1 | -1 (1.10056) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97770 HOMO: -7.35252 LUMO: -1.78235 factor:1 | -1 (0.47127) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16557 HOMO: -7.25456 LUMO: -1.66806 factor:1 | -1 (0.28341) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92314 HOMO: -7.54844 LUMO: -1.07213 factor:1 | -1 (0.52583) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81595 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (0.63302) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97645 HOMO: -7.01782 LUMO: -1.60547 factor:1 | -1 (0.47253) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09714 HOMO: -7.21646 LUMO: -1.53472 factor:1 | -1 (1.35183) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03711 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (1.41186) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18274 HOMO: -6.78924 LUMO: 0.66396 factor:1 | -1 (1.26623) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94688 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (1.50210) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16873 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (1.28024) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29230 HOMO: -7.10489 LUMO: -1.30887 factor:1 | -1 (1.15667) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06818 HOMO: -7.05047 LUMO: 0.42722 factor:1 | -1 (1.38079) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -6.61237 LUMO: 1.30887 factor:1 | -1 (1.12516) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32392 HOMO: -7.05863 LUMO: 0.59049 factor:1 | -1 (1.12505) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33246 HOMO: -6.26406 LUMO: 0.78641 factor:1 | -1 (1.11651) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99673 HOMO: -6.70489 LUMO: 0.67756 factor:1 | -1 (1.45224) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83220 HOMO: -6.78652 LUMO: -0.94968 factor:1 | -1 (0.61677) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93138 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.51759) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96311 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.48586) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21961 HOMO: -7.07224 LUMO: 0.85988 factor:1 | -1 (0.22936) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61309 HOMO: -7.02326 LUMO: 1.10206 factor:1 | -1 (0.83588) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72425 HOMO: -6.71305 LUMO: 0.84627 factor:1 | -1 (0.72472) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05046 HOMO: -7.27360 LUMO: 0.88165 factor:1 | -1 (0.39851) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.84911 LUMO: 0.59865 factor:1 | -1 (0.34210) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94725 HOMO: -6.75114 LUMO: -2.49801 factor:1 | -1 (0.50172) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06056 HOMO: -6.97156 LUMO: 0.53606 factor:1 | -1 (0.38842) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94787 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.50110) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12141 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (1.32756) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12152 HOMO: -6.34025 LUMO: 0.50341 factor:1 | -1 (1.32745) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94160 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (1.50737) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17771 HOMO: -6.54978 LUMO: -1.00682 factor:1 | -1 (1.27126) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16944 HOMO: -6.82462 LUMO: -0.98777 factor:1 | -1 (1.27953) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01482 HOMO: -6.85455 LUMO: -0.68573 factor:1 | -1 (1.43415) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11053 HOMO: -7.55388 LUMO: -0.03265 factor:1 | -1 (1.33845) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15406 HOMO: -6.77019 LUMO: -0.71838 factor:1 | -1 (1.29491) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37303 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (1.07594) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44563 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (1.00334) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22470 HOMO: -6.80829 LUMO: -0.77280 factor:1 | -1 (1.22427) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27466 HOMO: -6.94162 LUMO: -0.94151 factor:1 | -1 (1.17431) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06252 HOMO: -6.89809 LUMO: -0.90886 factor:1 | -1 (1.38645) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06952 HOMO: -6.85183 LUMO: -0.88981 factor:1 | -1 (1.37945) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27730 HOMO: -6.51985 LUMO: -0.84627 factor:1 | -1 (1.17167) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12530 HOMO: -6.83278 LUMO: -1.08029 factor:1 | -1 (1.32367) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28242 HOMO: -6.91986 LUMO: 0.66396 factor:1 | -1 (1.16655) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95452 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (1.49445) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92567 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (0.52330) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84559 HOMO: -6.74298 LUMO: -0.81634 factor:1 | -1 (0.60339) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37127 HOMO: -7.04503 LUMO: 1.15921 factor:1 | -1 (1.07771) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80148 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (0.64749) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93666 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (0.51231) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74569 HOMO: -7.12666 LUMO: 0.60681 factor:1 | -1 (0.70328) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10067 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (0.34831) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09189 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (1.35709) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83479 HOMO: -6.57427 LUMO: 0.71294 factor:1 | -1 (1.61418) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07235 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (1.37662) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26324 HOMO: -6.83550 LUMO: -0.77825 factor:1 | -1 (1.18574) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29662 HOMO: -7.14843 LUMO: 0.44627 factor:1 | -1 (1.15235) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02228 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (1.42669) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07678 HOMO: -6.81373 LUMO: -0.93879 factor:1 | -1 (1.37219) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21232 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (1.23665) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24008 HOMO: -7.13483 LUMO: -1.25444 factor:1 | -1 (1.20889) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15779 HOMO: -6.37835 LUMO: -1.54289 factor:1 | -1 (1.29118) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59576 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (0.85321) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63203 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (0.81694) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87771 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (1.57127) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76698 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (1.68199) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.79308 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (1.65589) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32316 HOMO: -6.35658 LUMO: -0.24218 factor:1 | -1 (1.12582) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13616 HOMO: -6.48175 LUMO: -0.71566 factor:1 | -1 (1.31281) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56362 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (0.88535) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35080 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (1.09817) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71799 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (0.73098) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56926 HOMO: -6.51441 LUMO: -0.65307 factor:1 | -1 (0.87972) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62542 HOMO: -6.57971 LUMO: -0.92519 factor:1 | -1 (0.82355) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87593 HOMO: -6.67223 LUMO: -0.58232 factor:1 | -1 (0.57304) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60283 HOMO: -6.10351 LUMO: -0.45987 factor:1 | -1 (0.84614) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92858 HOMO: -6.13889 LUMO: -0.50341 factor:1 | -1 (0.52039) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69971 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (0.74927) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28453 HOMO: -6.37563 LUMO: -0.22858 factor:1 | -1 (0.16444) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35683 HOMO: -6.37019 LUMO: 0.11429 factor:1 | -1 (0.09214) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48791 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-0.03894) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26780 HOMO: -6.41372 LUMO: -0.53879 factor:1 | -1 (0.18117) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08396 HOMO: -7.06680 LUMO: 0.32654 factor:1 | -1 (0.36501) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86955 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.42058) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76193 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.31296) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80563 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.35666) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57523 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-0.12626) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08512 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.63615) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57212 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.12315) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59425 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.14527) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52029 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-0.07132) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24735 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-0.79838) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54334 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-0.09437) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34265 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-0.89368) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03869 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.58972) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38360 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.93463) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09260 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-0.64363) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85608 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.40711) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88082 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.43184) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56136 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-0.11238) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69792 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.24895) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72524 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.27627) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79396 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-0.34499) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70152 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-0.25255) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75580 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-1.30683) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53906 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-1.09009) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10088 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.34809) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -6.42733 LUMO: -1.15648 factor:1 | -1 (0.52317) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96781 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-0.51884) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80639 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-0.35742) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00760 HOMO: -6.98788 LUMO: 0.34831 factor:1 | -1 (0.44137) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85057 HOMO: -6.80013 LUMO: -1.11567 factor:1 | -1 (0.59841) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80172 HOMO: -6.67767 LUMO: -0.82450 factor:1 | -1 (0.64725) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54389 HOMO: -6.84911 LUMO: -0.21497 factor:1 | -1 (0.90508) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88797 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.43900) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77407 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.32509) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38418 HOMO: -7.04503 LUMO: -1.04220 factor:1 | -1 (0.06479) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99304 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.54406) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87694 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.42797) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42923 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.98025) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50983 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.06085) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39972 HOMO: -6.58788 LUMO: -0.29116 factor:1 | -1 (0.04925) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51698 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-2.06801) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12507 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.67609) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33674 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.88777) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38238 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.93340) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07374 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.62476) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40532 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.95634) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09581 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-1.64683) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56956 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.12059) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56886 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.11988) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71169 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.26272) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61152 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.16255) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47626 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.02728) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11948 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.67051) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18215 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-1.73317) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99833 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.54936) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85074 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.40177) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23603 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-1.78705) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20392 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.75494) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36703 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.91806) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55713 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.10816) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68538 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.23640) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60954 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.16057) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59367 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.14470) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68843 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-0.23946) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42877 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.97980) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44739 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.99841) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30050 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.85153) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48333 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-1.03436) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48080 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.03183) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58875 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-1.13978) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02896 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.57998) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67732 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-1.22835) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13322 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-1.68425) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99284 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-1.54387) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98938 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-1.54041) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06887 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-1.61989) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26116 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.18781) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00480 HOMO: -6.32937 LUMO: -1.89119 factor:1 | -1 (0.44417) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49729 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-1.04832) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13151 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.68253) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29099 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-1.84202) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52595 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.07698) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18629 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.73732) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49901 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-1.05003) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22061 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.77163) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42254 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.97357) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89131 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-1.44234) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93877 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-1.48980) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52586 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-1.07689) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52369 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-1.07471) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57232 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.12335) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28806 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.83909) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82794 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-1.37896) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47803 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-1.02905) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59743 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-1.14846) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22959 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-0.78061) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36621 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-0.91724) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44510 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-0.99613) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19693 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.74796) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88995 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-1.44098) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05395 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-1.60498) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90628 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.45731) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60458 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-2.15560) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01806 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-1.56909) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91637 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.46740) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73536 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.28639) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-0.15151) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61357 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.16460) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39212 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.94315) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32102 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.87204) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.77629) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21369 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.76472) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19810 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.74913) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.96151) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35990 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.91093) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81243 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-1.36345) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32134 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.87237) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-0.86812) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40250 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.04648) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39229 HOMO: -6.50080 LUMO: -0.71294 factor:1 | -1 (0.05668) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27441 HOMO: -6.59060 LUMO: -0.57960 factor:1 | -1 (0.17456) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30306 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.85408) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10626 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.65729) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34300 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.89403) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.71566) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17075 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.72178) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77017 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-1.32119) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31225 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.86328) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08463 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.63566) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20730 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.75833) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.74869) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74753 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-1.29855) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.54349 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-2.09451) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55219 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-2.10322) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56058 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-1.11161) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36391 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (0.08506) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08665 HOMO: -6.49808 LUMO: -0.51157 factor:1 | -1 (0.36232) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18452 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.73555) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87728 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.42831) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22186 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.77288) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06874 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.61977) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99755 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.54858) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71142 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-1.26245) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06708 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.61811) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15130 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.70233) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12278 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.67381) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44831 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.99934) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26084 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.81187) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40031 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.95134) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16827 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-1.71930) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22552 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-1.77655) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38062 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (0.06836) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34153 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.89256) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32330 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.87433) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35693 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.90796) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39307 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.94410) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35185 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.90287) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45634 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-1.00737) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61191 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.16294) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80185 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.35288) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40533 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.95636) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02438 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-1.57540) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27571 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.82674) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79009 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.34111) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42658 HOMO: -7.30898 LUMO: 0.26667 factor:1 | -1 (0.02239) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41155 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.96258) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02112 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.57215) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58537 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-1.13640) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63074 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.18177) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29485 HOMO: -6.63686 LUMO: -0.56055 factor:1 | -1 (0.15413) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23688 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.78791) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54434 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-1.09537) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89393 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.44496) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71417 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.26520) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29625 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.84728) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62412 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-1.17515) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12479 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-1.67581) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41756 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.96859) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85747 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.40850) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29012 HOMO: -6.07630 LUMO: 1.81500 factor:1 | -1 (1.15885) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22704 HOMO: -6.20964 LUMO: 1.81500 factor:1 | -1 (0.22194) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16821 HOMO: -6.15522 LUMO: 1.90752 factor:1 | -1 (0.28077) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04145 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (0.40752) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92634 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-0.47737) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04137 HOMO: -7.37156 LUMO: 0.24490 factor:1 | -1 (0.40760) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67475 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-0.22577) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10121 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.34776) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79302 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.34405) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07440 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-0.62543) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89482 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.44585) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09742 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-0.64845) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89589 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.44692) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48033 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-2.03136) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83365 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.38468) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63613 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.18716) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91453 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.46556) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92672 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.47775) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32521 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (0.12376) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56914 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.12017) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91902 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.47005) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87875 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.42978) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09268 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.64371) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23032 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.78135) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71635 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-0.26738) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72909 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-0.28011) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29309 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.84412) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60343 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-2.15446) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.73846 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-2.28948) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19502 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.74605) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17611 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.72713) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08515 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-0.63617) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48301 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.03404) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40886 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.04011) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23591 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (0.21307) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26175 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-0.81278) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80111 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-0.35214) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34771 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-0.89874) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25062 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-0.80165) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29404 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.84507) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.75234) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13143 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-1.68245) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85327 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.40430) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26847 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.81950) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24063 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-0.79166) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58242 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-0.13344) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69906 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.25009) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65072 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-0.20175) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96166 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-0.51269) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07312 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-0.62415) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25854 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-0.80957) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90917 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.46020) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21843 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-0.76946) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17673 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.72776) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11730 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-1.66833) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95919 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.51021) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03582 HOMO: -6.83550 LUMO: 0.87893 factor:1 | -1 (0.41315) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93909 HOMO: -7.06680 LUMO: 0.87621 factor:1 | -1 (0.50989) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57990 HOMO: -6.52257 LUMO: 0.81362 factor:1 | -1 (0.86908) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88252 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.43355) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02433 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-0.57536) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68546 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.23649) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61610 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-0.16713) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46687 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (1.98210) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04079 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.59182) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54377 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-1.09480) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65172 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-0.20275) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30423 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (0.14474) | 1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32588 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (1.12310) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16639 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (1.28258) | 1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31247 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-0.86350) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33857 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.88959) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35000 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.90102) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72596 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.27698) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46309 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-1.01411) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82185 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.37288) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52184 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.07287) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86566 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.41669) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25797 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.80899) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37938 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.93041) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-1.11964) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32651 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-0.87754) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61240 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-0.16343) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06463 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-0.61566) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16136 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (1.28762) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28985 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (1.15912) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12265 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.32632) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48944 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-0.04046) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03911 HOMO: -6.97428 LUMO: 0.70750 factor:1 | -1 (0.40986) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98430 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.53533) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18170 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.26727) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11811 HOMO: -6.43821 LUMO: -1.00410 factor:1 | -1 (0.33086) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63078 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.81819) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43010 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (1.01888) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26617 HOMO: -6.07086 LUMO: -1.39594 factor:1 | -1 (1.18280) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.46623 HOMO: -6.78108 LUMO: -1.54833 factor:1 | -1 (0.98274) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05082 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.39816) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69694 HOMO: -6.85183 LUMO: 1.06669 factor:1 | -1 (1.75203) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25292 HOMO: -6.98516 LUMO: 1.43948 factor:1 | -1 (1.19605) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23480 HOMO: -6.94162 LUMO: 0.79185 factor:1 | -1 (1.21417) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40894 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-0.95996) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56687 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.11790) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39408 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.94511) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55755 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-0.10857) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93147 HOMO: -6.63141 LUMO: -0.91430 factor:1 | -1 (0.51751) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52809 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.07912) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95723 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.50825) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41474 HOMO: -6.73754 LUMO: -0.71838 factor:1 | -1 (0.03423) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07043 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.62145) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31969 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.12928) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07575 HOMO: -6.82189 LUMO: -0.64763 factor:1 | -1 (1.37322) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40126 HOMO: -6.56883 LUMO: -0.51974 factor:1 | -1 (2.04771) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46828 HOMO: -6.97428 LUMO: -0.95512 factor:1 | -1 (1.98069) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.90525 HOMO: -6.70489 LUMO: -0.04082 factor:1 | -1 (2.54372) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16764 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (1.28133) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43834 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (1.01063) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33148 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (1.11749) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22763 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-0.77865) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38874 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-0.93977) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83437 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-0.38539) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50143 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.05245) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39367 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-0.94470) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45141 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-1.00244) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87135 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.42238) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34711 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-0.89814) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46766 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.01869) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65635 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-0.20738) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18606 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (0.26292) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98808 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-0.53911) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48935 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-0.04038) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18100 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (1.26797) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29048 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-0.84151) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40453 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-0.95556) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37176 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-0.92279) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99140 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-0.54243) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49480 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-0.04582) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11889 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-0.66992) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13423 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (1.31475) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22533 HOMO: -6.17971 LUMO: 1.71704 factor:1 | -1 (1.22364) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04311 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-0.59413) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12418 HOMO: -6.52801 LUMO: 1.56193 factor:1 | -1 (0.32480) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91500 HOMO: -6.55794 LUMO: 1.52384 factor:1 | -1 (0.53397) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18627 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (0.26270) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15142 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (1.29755) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19662 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (1.25235) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57109 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.12212) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18259 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-0.73362) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45802 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.00904) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61691 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-1.16794) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.37848 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-1.92950) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46173 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-1.01275) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56475 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-1.11578) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19192 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-1.74294) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08122 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-1.63225) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33459 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.88562) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58167 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-1.13270) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28174 HOMO: -6.29671 LUMO: -0.89525 factor:1 | -1 (1.16723) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05935 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.61038) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72681 HOMO: -6.56883 LUMO: -0.86260 factor:1 | -1 (0.72216) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99193 HOMO: -6.93074 LUMO: -0.27483 factor:1 | -1 (0.45704) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20847 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.75950) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99826 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.54929) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29489 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.84592) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.30073 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.85176) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18530 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-1.73633) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47351 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-1.02454) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40455 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.95558) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56405 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.11508) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20833 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-0.75936) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89188 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-1.44291) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49752 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-0.04855) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.70167) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10680 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-1.65783) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95298 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.50401) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51521 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-2.06624) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59181 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-2.14284) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14311 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.69414) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25244 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28594 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-0.83697) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28948 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-0.84051) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67189 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-0.22292) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77379 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-0.32482) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88240 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (0.56657) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45706 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-2.00809) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04201 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-1.59304) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24778 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-1.79881) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95459 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-0.50561) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20665 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.75767) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34959 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-0.90062) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02487 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.57589) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05598 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-0.60700) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32481 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.12417) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42785 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-0.97888) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87505 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-0.42608) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46273 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.01376) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42797 HOMO: -7.03686 LUMO: 0.46804 factor:1 | -1 (0.02101) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55482 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-0.10585) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29520 HOMO: -6.41917 LUMO: 0.19320 factor:1 | -1 (0.15377) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83974 HOMO: -6.61237 LUMO: -0.04354 factor:1 | -1 (0.60924) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32447 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.87550) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20213 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.75316) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17290 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-0.72393) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21734 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-0.76837) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54250 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.09353) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42268 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-0.97371) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76345 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.31448) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59553 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.14656) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53087 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.08190) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13609 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.68711) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58280 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.13383) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60453 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.15556) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10425 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.65528) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08106 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-1.63208) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35370 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-0.90472) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88289 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-0.43391) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07453 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-0.62556) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91799 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-0.46902) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76337 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.31440) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91233 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.46336) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27894 HOMO: -6.21780 LUMO: 2.09256 factor:1 | -1 (1.17004) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28977 HOMO: -6.28311 LUMO: 1.80411 factor:1 | -1 (1.15921) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18808 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (1.26089) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26555 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (1.18342) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22517 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (1.22380) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90290 HOMO: -6.77291 LUMO: 1.89935 factor:1 | -1 (1.54607) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13507 HOMO: -6.36474 LUMO: 1.61091 factor:1 | -1 (1.31390) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10936 HOMO: -6.60420 LUMO: 1.40955 factor:1 | -1 (1.33962) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99776 HOMO: -6.81645 LUMO: 1.59731 factor:1 | -1 (1.45121) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34077 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.89180) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26774 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-0.81876) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32072 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-0.87174) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44616 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.99719) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31778 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-0.86881) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40401 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.95504) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64838 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-0.19941) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86645 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-0.41748) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26655 HOMO: -6.70489 LUMO: 1.78779 factor:1 | -1 (0.18243) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39353 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-0.94456) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29576 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-0.84679) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95354 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-1.50457) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15859 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-0.70962) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14616 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-0.69718) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78884 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.33987) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40583 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.95686) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32730 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-0.87833) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59857 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.14960) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22520 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-1.77622) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91112 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.46215) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03150 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-1.58253) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04445 HOMO: -6.86815 LUMO: 2.02997 factor:1 | -1 (0.40452) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95639 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.49258) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70737 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.25840) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02227 HOMO: -6.44638 LUMO: 2.16058 factor:1 | -1 (0.42670) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39964 HOMO: -6.65591 LUMO: 1.95106 factor:1 | -1 (0.04933) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81456 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.36558) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10796 HOMO: -6.48719 LUMO: 1.59187 factor:1 | -1 (0.34101) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63088 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.18191) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90197 HOMO: -6.92258 LUMO: 1.87214 factor:1 | -1 (0.54700) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68443 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.23546) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05599 HOMO: -6.27767 LUMO: 1.75513 factor:1 | -1 (0.39299) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88833 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.43936) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08829 HOMO: -6.62053 LUMO: 1.39594 factor:1 | -1 (0.36069) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42554 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (0.02343) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89679 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.44782) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76043 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.31146) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85233 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.40335) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31614 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-0.86717) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24036 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.79139) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20363 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.75465) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62659 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-2.17762) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58303 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-2.13405) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61824 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-2.16926) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25069 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-1.80172) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60108 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-0.15211) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24110 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.79212) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80709 HOMO: -6.47903 LUMO: -2.16875 factor:1 | -1 (1.64188) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27601 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.82704) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17837 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.72940) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84222 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.39325) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96844 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.51947) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34428 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.89531) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33133 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.88236) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69936 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-1.25039) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01410 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-0.56513) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32772 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (0.12125) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91815 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.46918) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84490 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-0.39593) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46813 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-0.01916) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32777 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.12120) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-0.78527) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21448 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-0.76551) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14776 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-0.69879) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15124 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.70227) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90947 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-0.46050) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33721 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-0.88823) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31620 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-0.86723) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05798 HOMO: -6.02188 LUMO: 1.91296 factor:1 | -1 (1.39099) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83379 HOMO: -6.17698 LUMO: 2.00004 factor:1 | -1 (1.61519) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03261 HOMO: -6.02732 LUMO: 1.90752 factor:1 | -1 (0.41636) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28121 HOMO: -6.68584 LUMO: -0.50885 factor:1 | -1 (0.16776) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88871 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.43974) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76577 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.31679) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90763 HOMO: -6.56339 LUMO: 0.23130 factor:1 | -1 (0.54134) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93928 HOMO: -6.76747 LUMO: 0.08980 factor:1 | -1 (0.50970) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81458 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.36561) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64138 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-0.19241) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69145 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-0.24248) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68992 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.24095) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91232 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.46335) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10942 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-0.66045) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10528 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.65631) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12670 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-0.67773) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20532 HOMO: -6.72938 LUMO: -0.64763 factor:1 | -1 (0.24365) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22957 HOMO: -6.49264 LUMO: -0.74559 factor:1 | -1 (0.21941) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80365 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.35467) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20712 HOMO: -6.33481 LUMO: 0.33198 factor:1 | -1 (0.24185) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97222 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-0.52325) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09429 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-0.64532) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20402 HOMO: -6.09263 LUMO: 0.21497 factor:1 | -1 (0.24496) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24799 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.20098) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45441 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-0.00544) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84090 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-0.39193) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20804 HOMO: -7.07768 LUMO: 0.28844 factor:1 | -1 (0.24093) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53135 HOMO: -6.75114 LUMO: 0.18776 factor:1 | -1 (0.91762) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83669 HOMO: -6.77019 LUMO: -0.12245 factor:1 | -1 (0.61228) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07894 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-0.62997) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85535 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-0.40637) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16701 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.28196) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05569 HOMO: -6.34297 LUMO: -0.33198 factor:1 | -1 (0.39329) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59764 HOMO: -7.51578 LUMO: 0.02177 factor:1 | -1 (0.85134) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26721 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.81824) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51599 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.06701) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22079 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.77181) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22125 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.77228) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53743 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.08846) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97954 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-0.53057) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96212 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-0.51315) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11261 HOMO: -6.52257 LUMO: -0.77280 factor:1 | -1 (0.33636) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51686 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.06789) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69772 HOMO: -6.08447 LUMO: 0.25851 factor:1 | -1 (0.75125) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11125 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.33772) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99669 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.45228) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21692 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.76795) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18732 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.73834) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-0.98587) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37035 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-0.92138) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11692 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.66795) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86164 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (0.58733) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73241 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-0.28343) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97914 HOMO: -6.89809 LUMO: 0.34558 factor:1 | -1 (0.46983) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18261 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.73364) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21145 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.76248) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35974 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-0.91077) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23476 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.78578) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86739 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-1.41842) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89505 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.44608) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05340 HOMO: -6.68312 LUMO: 1.69255 factor:1 | -1 (0.39557) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45545 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.00648) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87606 HOMO: -6.17971 LUMO: 1.90208 factor:1 | -1 (0.57291) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09052 HOMO: -6.53073 LUMO: 1.73337 factor:1 | -1 (0.35846) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98212 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.53315) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05272 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (0.39625) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94364 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.49467) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13369 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-0.68472) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85839 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.40941) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01576 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.56679) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64974 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.20077) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86315 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-1.41418) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97467 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.52570) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71474 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.26576) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.55400 HOMO: -6.41644 LUMO: 2.70209 factor:1 | -1 (1.89497) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76175 HOMO: -6.29671 LUMO: 2.14698 factor:1 | -1 (0.68722) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50044 HOMO: -6.29127 LUMO: 1.87486 factor:1 | -1 (0.94853) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61963 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.17066) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12343 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.67446) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69836 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.24938) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28771 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-0.83874) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42878 HOMO: -6.63414 LUMO: 1.62452 factor:1 | -1 (0.02019) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18502 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.26395) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33984 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (1.10914) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14395 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.69498) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14391 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.30507) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83595 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.38697) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23805 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.78908) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30366 HOMO: -6.65591 LUMO: 1.69527 factor:1 | -1 (0.14531) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05132 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-0.60235) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14976 HOMO: -6.68312 LUMO: 2.38100 factor:1 | -1 (0.29922) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91545 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-1.46648) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.31804 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.86907) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10254 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-0.65356) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30828 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.85931) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65275 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.20378) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34401 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.89504) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15521 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.70624) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82962 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.38065) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47463 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.02566) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39918 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (1.04979) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34585 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (1.10312) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21040 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.76143) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35917 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.08980) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24926 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-0.80029) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48342 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-0.03445) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88465 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-0.43568) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33440 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-0.88543) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50096 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-2.05198) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48741 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-1.03844) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41268 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-1.96371) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80342 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.35445) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19413 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.74516) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91186 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-1.46288) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48714 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.03817) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20430 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-1.75532) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40970 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.96073) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.88045) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97590 HOMO: -7.03959 LUMO: 1.27349 factor:1 | -1 (0.47307) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11610 HOMO: -6.67495 LUMO: -0.89253 factor:1 | -1 (0.33288) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85676 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.40779) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99497 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.54600) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87799 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.42901) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19143 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.74246) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66078 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.21180) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94437 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.49540) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10313 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-0.65416) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18266 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.73369) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34613 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.89716) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23067 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.78170) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87020 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.42123) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23053 HOMO: -6.90353 LUMO: 2.19868 factor:1 | -1 (1.21844) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91873 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (0.53024) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98747 HOMO: -6.46543 LUMO: 1.90752 factor:1 | -1 (0.46151) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02002 HOMO: -6.55522 LUMO: 2.11977 factor:1 | -1 (1.42895) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23739 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.78842) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56652 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.11754) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75551 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.30654) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15837 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.70940) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84795 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.39897) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90439 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.54458) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22848 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (0.22049) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01925 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (0.42972) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13911 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-0.69014) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33213 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.11685) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93345 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.51552) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03988 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (0.40910) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89857 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (0.55040) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04945 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-0.60047) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16772 HOMO: -5.98378 LUMO: 2.16331 factor:1 | -1 (0.28126) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91530 HOMO: -6.08991 LUMO: 2.30208 factor:1 | -1 (0.53367) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07951 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.63054) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11169 HOMO: -6.84638 LUMO: 1.76874 factor:1 | -1 (0.33729) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76381 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.31484) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67865 HOMO: -6.69672 LUMO: 1.71976 factor:1 | -1 (0.77033) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56988 HOMO: -6.86543 LUMO: 2.24766 factor:1 | -1 (0.87909) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82227 HOMO: -7.21646 LUMO: 1.71976 factor:1 | -1 (0.62671) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76356 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-0.31459) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67567 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.22670) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49193 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.04296) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87818 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-0.42921) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58193 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.13295) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51027 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.06130) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15937 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.71040) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46986 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.02089) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99442 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.54544) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30687 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-0.85789) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41778 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.96881) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17616 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.72719) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42188 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.97291) | 1 | 1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53786 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.08889) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60565 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.15667) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50001 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.05104) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41197 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (1.03700) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54894 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-1.09997) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16841 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-0.71944) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26625 HOMO: -6.83278 LUMO: 1.83949 factor:1 | -1 (0.18272) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61645 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.16748) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59185 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-1.14288) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38218 HOMO: -6.57155 LUMO: 1.89119 factor:1 | -1 (1.06680) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44733 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.99836) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06987 HOMO: -6.44638 LUMO: 2.26943 factor:1 | -1 (1.37910) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88524 HOMO: -5.88038 LUMO: 1.90480 factor:1 | -1 (1.56373) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31586 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (1.13311) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92588 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.47691) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18714 HOMO: -6.44366 LUMO: 2.24766 factor:1 | -1 (0.26183) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97948 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (1.46950) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39869 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (1.05028) | -1 | -1 |
| G: -5717.08328 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71898 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.27001) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23348 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-0.78450) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30989 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-0.86091) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25359 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-0.80461) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04606 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (1.40291) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83213 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (1.61685) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29966 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.14931) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95464 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-0.50567) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04796 HOMO: -6.69944 LUMO: 0.01905 factor:1 | -1 (0.40101) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73859 HOMO: -6.28583 LUMO: 0.38368 factor:1 | -1 (0.71038) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48553 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (0.96345) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37834 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (1.07063) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (1.28070) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08424 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (1.36473) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35264 HOMO: -6.76747 LUMO: -0.22041 factor:1 | -1 (0.09633) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18825 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.73928) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02574 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-0.57677) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14342 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (0.30556) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08096 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.63198) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20192 HOMO: -6.70216 LUMO: 0.61226 factor:1 | -1 (0.24705) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11888 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (1.33009) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16253 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (1.28645) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73946 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.70951) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63413 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.81484) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95567 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (1.49331) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19428 HOMO: -6.81645 LUMO: -0.07347 factor:1 | -1 (1.25469) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49718 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (1.95179) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.18738 HOMO: -6.71033 LUMO: -0.26395 factor:1 | -1 (2.26159) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06731 HOMO: -6.70489 LUMO: -0.09252 factor:1 | -1 (1.38166) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65767 HOMO: -6.23685 LUMO: 0.39729 factor:1 | -1 (0.79131) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62218 HOMO: -6.69400 LUMO: -0.05442 factor:1 | -1 (0.82679) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87040 HOMO: -6.36202 LUMO: 0.09796 factor:1 | -1 (0.57857) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74635 HOMO: -6.54978 LUMO: 0.15510 factor:1 | -1 (0.70263) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40139 HOMO: -6.77836 LUMO: 0.25851 factor:1 | -1 (1.04758) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61100 HOMO: -5.70623 LUMO: 0.73471 factor:1 | -1 (0.83797) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99422 HOMO: -5.58378 LUMO: 0.89253 factor:1 | -1 (1.45475) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96243 HOMO: -5.68718 LUMO: 0.87893 factor:1 | -1 (0.48654) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85658 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.59239) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67560 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (0.77337) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61647 HOMO: -4.45450 LUMO: 1.82044 factor:1 | -1 (0.83251) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00529 HOMO: -4.64226 LUMO: 1.70615 factor:1 | -1 (0.44368) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14478 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.30420) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.34486 HOMO: -4.85723 LUMO: 0.93607 factor:1 | -1 (0.10411) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12491 HOMO: -4.72934 LUMO: 1.00410 factor:1 | -1 (0.32406) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92959 HOMO: -4.56335 LUMO: 1.56738 factor:1 | -1 (0.51938) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52689 HOMO: -5.48854 LUMO: 0.33198 factor:1 | -1 (0.92209) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45353 HOMO: -4.97424 LUMO: 1.33608 factor:1 | -1 (0.99545) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41206 HOMO: -4.60145 LUMO: 1.74697 factor:1 | -1 (1.03692) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32226 HOMO: -5.60010 LUMO: 0.74831 factor:1 | -1 (1.12671) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10074 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-0.65177) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64742 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.19844) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34318 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-1.89421) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76614 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.31717) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11750 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.66853) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01951 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-0.57054) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08723 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.63826) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07733 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.62836) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09491 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-1.64594) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38651 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-0.93754) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45819 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-1.00922) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05534 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-1.60637) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47415 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-2.02518) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19978 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-1.75081) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57245 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-1.12348) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21910 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-1.77013) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.65837 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-2.20940) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55163 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-1.10266) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85039 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-1.40141) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62621 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-2.17724) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52436 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.92462) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25452 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.19445) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28350 HOMO: -5.80147 LUMO: 0.72382 factor:1 | -1 (0.16547) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21687 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-1.76790) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65114 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-1.20217) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24718 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-1.79821) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82168 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-1.37271) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59957 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-2.15060) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15075 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-1.70177) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32414 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (1.12484) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41313 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.96415) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56369 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.11471) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71817 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.26919) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.11964) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66709 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-1.21812) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96698 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.48200) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47510 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.02612) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11151 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (1.33747) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43480 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (1.01417) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29515 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (0.15383) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38244 HOMO: -5.87766 LUMO: 0.42994 factor:1 | -1 (0.06653) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09753 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.64856) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31681 HOMO: -5.99739 LUMO: 0.69389 factor:1 | -1 (0.13217) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67216 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-0.22319) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19991 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (0.24907) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05121 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-1.60223) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.14049 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.69151) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09551 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.64653) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05489 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.60592) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27715 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-0.82818) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78053 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-1.33156) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78862 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.33965) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15248 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.29650) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11608 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (1.33290) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49955 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-1.05058) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58156 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.13259) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27476 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-0.82578) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37228 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.92331) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45160 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.00263) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43439 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.01459) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11205 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (1.33692) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24043 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (1.20854) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24035 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (1.20862) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16792 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-0.71895) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36726 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (0.08172) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21960 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.77063) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42573 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (0.02324) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10475 HOMO: -4.97696 LUMO: 0.89798 factor:1 | -1 (0.34422) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36859 HOMO: -5.00690 LUMO: 1.14288 factor:1 | -1 (0.08038) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19430 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (0.25467) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65698 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (0.79199) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59329 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.14432) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60576 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.15678) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55979 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-2.11081) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41783 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.96886) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16645 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-1.71747) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64192 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.19295) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05013 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.60115) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98783 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (1.46114) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98276 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (0.46621) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48344 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.03447) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57150 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-1.12252) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30175 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.85278) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.00440) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49101 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-1.04203) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27369 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.82472) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46358 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-1.01460) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72993 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.28096) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56937 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-1.12040) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41957 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (1.02941) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19559 HOMO: -6.54978 LUMO: 0.34831 factor:1 | -1 (1.25338) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36144 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (1.08753) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14567 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.69669) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47183 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.02286) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32119 HOMO: -7.39878 LUMO: 0.15783 factor:1 | -1 (0.12778) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43609 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.98712) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89977 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.45080) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52913 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.08016) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44891 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.99994) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17527 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.72630) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07513 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.62616) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70883 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.25986) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46227 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.01330) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31193 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.86295) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72627 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-1.27730) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00021 HOMO: -6.97156 LUMO: -0.53606 factor:1 | -1 (1.44876) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76315 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.31418) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.67340) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29158 HOMO: -7.49946 LUMO: -0.14694 factor:1 | -1 (0.15739) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05408 HOMO: -7.44231 LUMO: 0.58232 factor:1 | -1 (0.39489) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20297 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.75400) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33972 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.10925) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21609 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-0.76712) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26864 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.18033) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79576 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (0.65321) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08738 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.63841) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21234 HOMO: -7.47769 LUMO: -1.02859 factor:1 | -1 (0.23663) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01362 HOMO: -6.75659 LUMO: 0.39457 factor:1 | -1 (0.43535) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35159 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (1.09738) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41304 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.96407) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36385 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.91487) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17231 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-0.72333) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82854 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-1.37956) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48211 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-1.03313) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54567 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.09670) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45035 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-1.00138) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60684 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.15787) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17806 HOMO: -6.82189 LUMO: -1.15376 factor:1 | -1 (1.27091) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06337 HOMO: -6.65046 LUMO: -0.46531 factor:1 | -1 (1.38560) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00359 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.55462) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11699 HOMO: -6.80557 LUMO: 0.44355 factor:1 | -1 (0.33198) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17620 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.72722) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48124 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.03227) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81039 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-0.36142) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25233 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.80336) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33716 HOMO: -6.26406 LUMO: -1.09934 factor:1 | -1 (0.11181) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54614 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-0.09717) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54640 HOMO: -6.12256 LUMO: -0.42178 factor:1 | -1 (0.90257) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06527 HOMO: -6.09807 LUMO: 0.11429 factor:1 | -1 (1.38370) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24786 HOMO: -7.35252 LUMO: -0.55783 factor:1 | -1 (1.20111) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59723 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (0.85174) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40740 HOMO: -6.16066 LUMO: 0.01905 factor:1 | -1 (1.04157) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96932 HOMO: -6.13345 LUMO: -0.41906 factor:1 | -1 (0.47966) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74863 HOMO: -6.10351 LUMO: -0.33742 factor:1 | -1 (0.70034) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -7.24639 LUMO: -0.51702 factor:1 | -1 (0.52317) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60169 HOMO: -6.98244 LUMO: -1.82044 factor:1 | -1 (0.84728) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16401 HOMO: -6.37563 LUMO: -1.67622 factor:1 | -1 (0.28496) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76912 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (0.67985) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40155 HOMO: -6.34025 LUMO: -0.27483 factor:1 | -1 (1.04742) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86826 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (1.58071) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35842 HOMO: -7.53755 LUMO: -0.38912 factor:1 | -1 (1.09055) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85248 HOMO: -7.00421 LUMO: -0.50885 factor:1 | -1 (1.59649) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00446 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (1.44452) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21317 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (1.23581) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80954 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (1.63943) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92533 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (1.52365) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23722 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (1.21175) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89803 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (1.55094) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82959 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (0.61939) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96543 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.48355) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52041 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.92856) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59268 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (0.85629) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20765 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.75868) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73686 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-1.28789) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-0.72015) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12441 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-0.67544) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34866 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.89969) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18346 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.73449) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43057 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.98160) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35489 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.90592) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83690 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.38793) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24251 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.79354) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20281 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.75384) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.82674 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (1.62223) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46358 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.01461) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88357 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.56540) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05372 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.60475) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17920 HOMO: -6.71849 LUMO: -0.84355 factor:1 | -1 (0.26977) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32892 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (0.12006) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55826 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (0.89071) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.44610) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04491 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (0.40406) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28541 HOMO: -6.52801 LUMO: 0.98233 factor:1 | -1 (1.16356) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00726 HOMO: -6.76475 LUMO: 0.53334 factor:1 | -1 (1.44171) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41739 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (1.03158) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25504 HOMO: -6.57971 LUMO: 0.12789 factor:1 | -1 (0.19394) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86774 HOMO: -6.99333 LUMO: 0.51430 factor:1 | -1 (0.58124) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81707 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (0.63190) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57445 HOMO: -6.16066 LUMO: 1.77146 factor:1 | -1 (0.87452) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09841 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (0.35056) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36411 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (1.08486) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23709 HOMO: -6.60420 LUMO: 1.33880 factor:1 | -1 (1.21189) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16187 HOMO: -6.23957 LUMO: 0.09524 factor:1 | -1 (1.28710) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10478 HOMO: -6.80013 LUMO: 1.34696 factor:1 | -1 (1.34419) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31872 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (1.13025) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15710 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.29187) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52421 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-0.07524) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76760 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (0.68137) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22483 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.22414) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02524 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.42374) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36288 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (0.08610) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91389 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.53508) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40829 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (0.04068) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96420 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (0.48477) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59042 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.14144) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26048 HOMO: -7.96477 LUMO: -2.75651 factor:1 | -1 (0.18849) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63605 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-0.18708) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67651 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.22754) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36805 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (0.08093) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81331 HOMO: -8.07362 LUMO: -0.28028 factor:1 | -1 (0.63566) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75644 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.69253) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49386 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.04489) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26823 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.81925) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-0.44610) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13647 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.68750) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25125 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.80227) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22910 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.78012) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36779 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.91882) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06062 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-1.61165) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22752 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.77854) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81825 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.36928) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04797 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-1.59900) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17711 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-1.72814) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22319 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.77422) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37849 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.92951) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74102 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.29205) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86464 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-1.41567) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20443 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-1.75546) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92873 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-1.47976) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22496 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.77599) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08971 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-1.64074) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34243 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.89346) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23344 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-1.78447) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51740 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-1.06843) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34004 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-0.89106) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27138 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.82241) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08127 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-1.63230) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10685 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-1.65788) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39818 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-1.94921) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30591 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.85694) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35628 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-0.90731) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48502 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.03605) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.33527 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.88629) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07738 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.62841) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93841 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-1.48944) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33299 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.88402) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74962 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-1.30065) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35345 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.90448) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16885 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.71988) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28689 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.83792) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32613 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-0.87716) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21129 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-1.76232) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42681 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-0.97784) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90307 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.45409) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48227 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.03330) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18533 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-1.73636) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32865 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-1.87968) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75087 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-1.30190) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16977 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.72080) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98340 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-1.53442) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35536 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.90638) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43032 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.98135) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15938 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.71041) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96533 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-1.51635) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94126 HOMO: -7.33619 LUMO: -1.02587 factor:1 | -1 (0.50771) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10401 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (0.34496) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75798 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.30901) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12984 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.31914) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29681 HOMO: -7.43415 LUMO: 0.10612 factor:1 | -1 (0.15217) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04958 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.60061) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90445 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.45548) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00590 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-1.55693) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07863 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-1.62966) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15235 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.70338) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19339 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.74441) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04165 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.59268) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09844 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-1.64947) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86124 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.41227) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08653 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.63755) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86706 HOMO: -7.86137 LUMO: 0.01633 factor:1 | -1 (0.58192) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03433 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.41465) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01892 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (0.43005) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84461 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (0.60436) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73139 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.28242) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85701 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.40803) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82992 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.38095) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74554 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-1.29657) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92841 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.47944) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28741 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.83844) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15835 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.70937) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80032 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.35134) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97810 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-0.52913) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70740 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.25843) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64851 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.19954) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39903 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.95006) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48611 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-1.03713) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53988 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.09090) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59174 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.14277) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46943 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.02045) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53811 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.08914) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31364 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-0.86467) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33492 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.88595) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30810 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (0.14087) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36449 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (1.08448) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35543 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (1.09354) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50011 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.94886) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-0.72015) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40723 HOMO: -7.47225 LUMO: -0.22041 factor:1 | -1 (0.04174) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05638 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.60741) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24369 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (0.20528) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41464 HOMO: -6.52257 LUMO: -1.11022 factor:1 | -1 (1.03433) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42523 HOMO: -6.75114 LUMO: -1.09934 factor:1 | -1 (1.02375) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44662 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.99765) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89890 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-1.44993) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17821 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-0.72924) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30257 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-0.85359) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36093 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-0.91196) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87458 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.42560) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31976 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.87079) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36191 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-0.91294) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17658 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-0.72761) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37737 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-0.92840) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97384 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (1.47513) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93188 HOMO: -7.12938 LUMO: -0.23674 factor:1 | -1 (1.51709) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99932 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-0.55035) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06556 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.38341) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94700 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-0.49802) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09038 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.35859) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03457 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.41440) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99910 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.55013) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13588 HOMO: -5.62187 LUMO: 0.05714 factor:1 | -1 (0.31309) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86249 HOMO: -7.03414 LUMO: -1.04492 factor:1 | -1 (0.58649) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26328 HOMO: -6.75387 LUMO: -2.02181 factor:1 | -1 (0.18569) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07438 HOMO: -6.55250 LUMO: -0.75648 factor:1 | -1 (0.37459) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.61392) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11631 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (0.33266) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36671 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.08226) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90959 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.53938) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94575 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.50322) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00161 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-0.55264) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79333 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-0.34436) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.67661) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66492 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.21595) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77358 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.32460) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78076 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.33179) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07317 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-1.62419) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24950 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-0.80053) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28828 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-0.83931) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06051 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.61154) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25212 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.80314) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16495 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-1.71598) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11824 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.66926) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66848 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.21951) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49294 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.04396) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26771 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.81874) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27723 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-0.82826) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73683 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.28786) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12944 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-1.68047) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98645 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-0.53748) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89630 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-0.44733) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55977 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.11080) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13036 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-1.68139) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84081 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-1.39184) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61362 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-1.16465) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95470 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-0.50572) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49471 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.04573) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06749 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.61851) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75271 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.30373) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89260 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.44363) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07228 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.62330) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84441 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.39544) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92451 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.47554) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93458 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-1.48561) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91614 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.46717) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03554 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-0.58657) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17739 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-0.72842) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37579 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.92682) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79512 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-1.34615) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04889 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-1.59992) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70402 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-1.25504) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77265 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.32368) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64288 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-0.19391) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82334 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-1.37437) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04282 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.59385) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01303 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.56406) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93980 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.49083) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86715 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.41818) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01706 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.56808) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95771 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.50874) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81920 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.37023) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24035 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.79138) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11110 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.66213) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92978 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (0.51919) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87748 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (0.57149) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71111 HOMO: -5.98106 LUMO: -0.37824 factor:1 | -1 (0.73786) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61315 HOMO: -7.06408 LUMO: -1.12927 factor:1 | -1 (0.83582) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15103 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.70205) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60309 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-1.15412) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79287 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.34390) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73547 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-1.28650) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88103 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.43206) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84154 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.39257) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01437 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-0.56540) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97032 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (0.47865) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91770 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (0.53128) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10614 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (0.34284) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53315 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (0.91583) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76605 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (0.68292) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27266 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-0.82369) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77137 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.32240) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90055 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-0.45157) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69262 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.24365) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45055 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.00158) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49305 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.04408) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52805 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.07908) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06945 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.62047) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83420 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.38522) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24487 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.79590) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.78527) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17548 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-1.72651) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46156 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.01259) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86310 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.41413) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56981 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.12084) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83292 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.38395) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71476 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.26579) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96637 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.51740) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16330 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.71433) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29010 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.84113) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61077 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.16180) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93422 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-1.48525) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99883 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.54986) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07168 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.62271) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11581 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.66684) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.69672 LUMO: -1.05036 factor:1 | -1 (0.52741) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88586 HOMO: -6.78924 LUMO: -1.03675 factor:1 | -1 (0.56311) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99762 HOMO: -6.81373 LUMO: -0.85988 factor:1 | -1 (0.45136) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49267 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.04369) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67140 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.22243) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.09695) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85500 HOMO: -7.17020 LUMO: 0.04898 factor:1 | -1 (0.59397) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62950 HOMO: -7.16476 LUMO: 0.04898 factor:1 | -1 (0.81947) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83593 HOMO: -6.59332 LUMO: -0.49253 factor:1 | -1 (0.61305) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64104 HOMO: -7.46953 LUMO: 0.84083 factor:1 | -1 (0.80793) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45273 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.00376) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49270 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.04373) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58546 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.13649) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79186 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.34289) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55531 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.10634) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11851 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.66954) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64916 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.20019) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91742 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.46844) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51729 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.06832) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80854 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.35957) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59177 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.14280) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.49664) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82370 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.37473) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94590 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.49693) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43783 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.98886) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54877 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-1.09980) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48132 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-1.03235) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08628 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-1.63731) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06531 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.61634) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20605 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.75708) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63809 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-0.18912) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43528 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (0.01369) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32308 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-0.87411) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19202 HOMO: -7.01510 LUMO: -1.64085 factor:1 | -1 (0.25696) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24617 HOMO: -6.59876 LUMO: -0.91158 factor:1 | -1 (0.20281) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53770 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-1.08873) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22293 HOMO: -6.70489 LUMO: -0.65579 factor:1 | -1 (0.22604) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23533 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.78635) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16564 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.71667) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70157 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.25259) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87978 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.43081) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30004 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.85106) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83361 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-0.38463) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35021 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.90124) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52009 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.07112) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76838 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.31941) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29233 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-0.84336) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49846 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-1.04949) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27277 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.82380) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13464 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-0.68567) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04751 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-0.59854) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92789 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.47892) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61254 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.16357) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17277 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-0.72380) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10449 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.65552) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26578 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.81680) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93731 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.48834) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36864 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.91966) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32970 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.88072) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19758 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-0.74861) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89891 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-0.44994) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00512 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.55615) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82694 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.37797) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55836 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.10939) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59083 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.14185) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95303 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-1.50405) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00272 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.55375) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29906 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-0.85008) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00466 HOMO: -6.55794 LUMO: 0.05170 factor:1 | -1 (0.44431) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99627 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.54730) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01852 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (0.43046) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96186 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (0.48711) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93759 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.51138) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11566 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (0.33331) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08208 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.36689) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19392 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.25505) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06780 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.38118) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00134 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-0.55236) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64519 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.19622) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95146 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-0.50249) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06331 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (0.38567) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28478 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (0.16419) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94080 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (0.50817) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00856 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (0.44042) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94804 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.50093) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83119 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (0.61778) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30112 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.85215) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90673 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.54224) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88933 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.44036) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04617 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-1.59720) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41562 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-1.96665) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09200 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-1.64302) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60504 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-2.15607) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24283 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-1.79386) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48305 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-2.03408) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35066 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.09831) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.24539) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55765 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.10868) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79080 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.34183) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09943 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-0.65046) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25669 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-0.80772) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93170 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-0.48273) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72492 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-0.27595) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.73800) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32218 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-1.87320) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41626 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.96728) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86078 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.41181) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07698 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.62800) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42560 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (0.02337) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33996 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (0.10901) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39813 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.94916) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50265 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-1.05368) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.96151) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87393 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.42496) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09211 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.64314) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26921 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.82023) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39223 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.94326) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03946 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.59049) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44279 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.99381) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08643 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.63745) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60595 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.15698) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50481 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.05584) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94147 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.49250) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31688 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.86791) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04262 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.59364) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23541 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.78644) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00321 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.55424) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86555 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-0.41658) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35898 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.08999) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39326 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-0.94429) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79524 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-0.34626) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25672 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-0.80774) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22218 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-0.77321) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19141 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.74244) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35860 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.09037) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42045 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.97147) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40605 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.95708) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13005 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.68107) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55547 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.10650) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95361 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.50464) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.15151) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40132 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.95234) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34523 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-0.89626) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11913 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.67016) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-0.88045) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29217 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.84320) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46582 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-0.01684) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36666 HOMO: -6.92530 LUMO: -0.88165 factor:1 | -1 (0.08231) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42072 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-0.97175) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18882 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.73985) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26221 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.81324) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89932 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-0.45035) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94106 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.49209) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64429 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.19531) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93931 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-1.49034) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78456 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-1.33559) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.28261 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-1.83364) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90976 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.46079) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29409 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-1.84512) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47143 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-2.02246) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.78221 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-2.33324) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05172 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.60275) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22778 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.77881) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18998 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.74101) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52299 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-0.07401) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25413 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.80516) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19625 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-0.74728) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32295 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.87398) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27122 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-0.82225) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67419 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.22522) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04286 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.59389) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62450 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.17553) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20997 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.76099) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14798 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.69901) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20151 HOMO: -6.72938 LUMO: 0.30749 factor:1 | -1 (0.24746) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50639 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.05742) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18700 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-0.73803) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15125 HOMO: -6.38379 LUMO: -0.76736 factor:1 | -1 (0.29772) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12145 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-0.67247) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30069 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.85172) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60921 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.16024) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69344 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-0.24447) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08409 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-0.63511) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70356 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-0.25459) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58135 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-1.13237) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12656 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-0.67759) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23881 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-0.78984) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04087 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.59190) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75678 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.30781) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68148 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.23251) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28042 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-0.83144) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26287 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.18610) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31119 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.86222) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.63650 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.18752) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.66539 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-2.21642) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70127 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.25230) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62490 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-2.17593) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51660 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-2.06763) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17960 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.73063) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09726 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-0.64828) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11894 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.66997) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88234 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.43337) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61286 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-1.16389) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95513 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.50616) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78525 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.33628) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82220 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-0.37323) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56197 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.11300) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15421 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-0.70524) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22012 HOMO: -7.47769 LUMO: 0.40817 factor:1 | -1 (0.22885) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20137 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.75239) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17451 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-0.72554) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26414 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-1.81516) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41661 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.96764) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.74869) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13243 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-1.68346) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09341 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-1.64444) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17383 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.72486) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90629 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.45731) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47010 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-2.02113) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22759 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.77862) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60578 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.15681) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10613 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-0.65715) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01255 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-0.56358) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18545 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.73648) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80411 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.35514) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13062 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.68165) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91570 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.46673) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06610 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.61713) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77009 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.32112) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71815 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.26918) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22624 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.77727) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18623 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-1.73726) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19002 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.74105) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90191 HOMO: -7.01237 LUMO: 0.02721 factor:1 | -1 (0.54706) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73285 HOMO: -6.39195 LUMO: 1.46941 factor:1 | -1 (0.71612) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13267 HOMO: -6.53890 LUMO: 1.32792 factor:1 | -1 (0.31631) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82746 HOMO: -6.82734 LUMO: 1.98099 factor:1 | -1 (0.62151) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00351 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.55454) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12243 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.67345) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85510 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.40613) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79520 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-1.34623) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04387 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.59490) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29040 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.84143) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36527 HOMO: -6.77564 LUMO: 0.42178 factor:1 | -1 (0.08370) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20287 HOMO: -6.56339 LUMO: 1.65717 factor:1 | -1 (0.24610) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47960 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.03063) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18611 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.26286) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19835 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.74937) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45154 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-2.00257) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07129 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.62232) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40614 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (0.04283) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59768 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-0.14871) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59942 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.15045) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73379 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.28482) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.29900) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07887 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.37010) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.13429) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40525 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.95628) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99025 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.54128) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84932 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.40035) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96656 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-0.51759) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95285 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-0.50387) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08240 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.63343) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85845 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.40948) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08180 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-0.63283) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98593 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.53696) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17201 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.72303) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96768 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.51870) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99368 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.54471) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64084 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.19187) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92346 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.47448) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14275 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.69378) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13206 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-0.68309) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75181 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.30284) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65670 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-0.20773) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75736 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.30839) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44228 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (0.00669) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11376 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.33522) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30892 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (0.14006) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (0.61392) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.12338 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (2.32559) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26732 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (1.18165) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12269 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (1.32628) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23892 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-0.78995) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39130 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-0.94233) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96237 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-0.51340) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05121 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (2.39776) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96481 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (1.48416) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73298 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.28401) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29495 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.84597) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30617 HOMO: -6.38379 LUMO: 0.45443 factor:1 | -1 (0.14281) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90060 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.45163) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47683 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-1.02786) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56753 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.11856) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16556 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.71658) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43262 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (0.01635) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09117 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (0.35780) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96494 HOMO: -6.70489 LUMO: 0.19048 factor:1 | -1 (0.48404) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67654 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.22757) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20908 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (0.23990) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22306 HOMO: -6.77564 LUMO: 0.72382 factor:1 | -1 (0.22591) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.57849) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05265 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (1.39633) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05218 HOMO: -7.09945 LUMO: 0.33470 factor:1 | -1 (1.39679) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89689 HOMO: -7.20830 LUMO: 0.59593 factor:1 | -1 (1.55208) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04030 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.59133) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21535 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.76638) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90406 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.45508) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26722 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.81825) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60438 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.15540) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36135 HOMO: -7.27360 LUMO: 0.42178 factor:1 | -1 (0.08762) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46875 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-1.01977) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43715 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.98818) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78737 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.33840) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45461 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.00563) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91004 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.46107) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13622 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.68725) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47477 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.02580) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20091 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.24806) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99151 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.54254) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21549 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.76652) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88778 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.43881) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60114 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.15217) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50423 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-1.05526) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13885 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-1.68988) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.98587) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74969 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.30071) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09100 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.64203) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89529 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.44632) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90729 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.45832) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11723 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-0.66826) | 1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82898 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.38001) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59627 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.14730) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96691 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.51794) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69096 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-0.24199) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43586 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (0.01312) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05859 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.60962) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33354 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.11543) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17615 HOMO: -6.90353 LUMO: -0.64763 factor:1 | -1 (0.27282) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20874 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.75977) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17331 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.72434) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06956 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.62058) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00528 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.55631) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08355 HOMO: -6.52529 LUMO: 1.58914 factor:1 | -1 (0.36542) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13217 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.68320) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29002 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.84105) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77457 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (1.67440) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81681 HOMO: -6.75387 LUMO: 0.14422 factor:1 | -1 (1.63217) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73966 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (1.70931) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29337 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.84440) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21704 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-0.76807) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13306 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-1.68409) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53301 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-2.08404) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71504 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.26606) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74442 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-1.29545) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05462 HOMO: -7.31986 LUMO: 0.48708 factor:1 | -1 (0.39435) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91179 HOMO: -6.76475 LUMO: -0.75648 factor:1 | -1 (0.53718) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89487 HOMO: -6.76747 LUMO: -1.06941 factor:1 | -1 (0.55411) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97147 HOMO: -6.87087 LUMO: 0.72927 factor:1 | -1 (0.47751) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69238 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.24341) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69690 HOMO: -6.54706 LUMO: -0.03265 factor:1 | -1 (0.75207) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45415 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (0.99482) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70986 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (0.73912) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60209 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.15312) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93974 HOMO: -6.67223 LUMO: 0.03537 factor:1 | -1 (0.50923) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04305 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.59408) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93146 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.48249) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19673 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.74776) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25159 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.80262) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47675 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.02777) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05600 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-1.60702) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92585 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.47688) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15440 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.70543) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86065 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.41168) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82697 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.37799) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96082 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.51185) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71578 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.26681) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74573 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.29676) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78683 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.33786) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90819 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.45922) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72201 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.27304) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83921 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.39024) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71847 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.26950) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85605 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.40708) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97034 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.52137) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05476 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (0.39421) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76610 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.68287) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79592 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.34695) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56768 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (0.88130) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92736 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (0.52162) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87089 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (0.57808) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10922 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-1.66025) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27646 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-1.82749) | 1 | 1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39647 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.94750) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88889 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-1.43992) | -1 | -1 |
| G: -5717.08328 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94335 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.49438) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04254 HOMO: -8.21240 LUMO: 0.05987 factor:1 | -1 (0.40643) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68166 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.23268) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69010 HOMO: -6.80829 LUMO: -0.29933 factor:1 | -1 (0.75887) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00921 HOMO: -6.84094 LUMO: -0.53606 factor:1 | -1 (0.43976) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92847 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (0.52050) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93187 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.48289) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12244 HOMO: -6.39468 LUMO: -1.06941 factor:1 | -1 (0.32654) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90783 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-1.45886) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07772 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.62875) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67888 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.22991) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96539 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.51642) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92892 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.47995) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99045 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.54148) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86667 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.41769) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75545 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-1.30647) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67447 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.22550) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01914 HOMO: -5.05588 LUMO: 1.02859 factor:1 | -1 (0.42983) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48151 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.03254) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92433 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.47536) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52992 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.08095) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51816 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-1.06919) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94838 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.49941) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37618 HOMO: -5.56473 LUMO: 0.32109 factor:1 | -1 (0.07279) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31389 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-0.86491) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23122 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.78225) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65406 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.20509) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13205 HOMO: -4.44906 LUMO: 1.37690 factor:1 | -1 (1.31692) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.20722 HOMO: -4.62049 LUMO: 1.34968 factor:1 | -1 (2.24176) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.22316 HOMO: -4.59600 LUMO: 1.58370 factor:1 | -1 (2.22581) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29914 HOMO: -4.98785 LUMO: 1.46669 factor:1 | -1 (2.14984) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67860 HOMO: -5.06676 LUMO: 1.27349 factor:1 | -1 (1.77037) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.94659 HOMO: -5.09125 LUMO: 1.13471 factor:1 | -1 (2.50239) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.02572 HOMO: -4.84635 LUMO: 1.33608 factor:1 | -1 (2.42326) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14808 HOMO: -4.94431 LUMO: 1.18370 factor:1 | -1 (1.30089) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21300 HOMO: -4.92526 LUMO: 1.39867 factor:1 | -1 (1.23597) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39450 HOMO: -5.71983 LUMO: 0.60137 factor:1 | -1 (1.05447) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26816 HOMO: -5.10486 LUMO: 1.05580 factor:1 | -1 (1.18081) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36370 HOMO: -5.20282 LUMO: 1.01226 factor:1 | -1 (1.08527) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04699 HOMO: -4.98513 LUMO: 1.53744 factor:1 | -1 (1.40199) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25701 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.80804) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96455 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.51557) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44635 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.99738) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-1.00440) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96335 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.51438) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62026 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.17129) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40172 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-0.95275) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68895 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.23998) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44227 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.99330) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41027 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.96130) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10983 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.66086) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79145 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.34248) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.49664) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08836 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.63939) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76688 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.31791) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35760 HOMO: -5.47221 LUMO: 0.97961 factor:1 | -1 (0.09138) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22936 HOMO: -5.06948 LUMO: 1.12111 factor:1 | -1 (1.21961) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55785 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.10887) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93061 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.48164) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94832 HOMO: -5.38513 LUMO: 0.49253 factor:1 | -1 (1.50065) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42597 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.97700) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53879 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.08982) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36958 HOMO: -5.17561 LUMO: 1.04492 factor:1 | -1 (1.07939) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49454 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.04557) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34736 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.89838) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-0.70167) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22073 HOMO: -5.79058 LUMO: 0.53879 factor:1 | -1 (1.22824) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33573 HOMO: -5.36881 LUMO: 1.56465 factor:1 | -1 (1.11325) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13665 HOMO: -4.67492 LUMO: 1.32792 factor:1 | -1 (1.31232) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01801 HOMO: -4.60145 LUMO: 1.19458 factor:1 | -1 (1.43097) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92909 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.48012) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06143 HOMO: -4.65043 LUMO: 1.34696 factor:1 | -1 (0.38754) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93228 HOMO: -4.77560 LUMO: 1.35241 factor:1 | -1 (0.51669) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25068 HOMO: -4.94431 LUMO: 1.17825 factor:1 | -1 (0.19829) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99094 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.54197) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17261 HOMO: -5.34432 LUMO: 1.16737 factor:1 | -1 (0.27636) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80479 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.35582) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82989 HOMO: -4.81369 LUMO: 1.14288 factor:1 | -1 (0.61909) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44784 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (1.00113) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41959 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (1.02938) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00805 HOMO: -5.00417 LUMO: 1.01226 factor:1 | -1 (1.44092) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93354 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (1.51543) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35034 HOMO: -5.51303 LUMO: 0.54151 factor:1 | -1 (1.09863) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28030 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (1.16867) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89065 HOMO: -4.79193 LUMO: 1.12111 factor:1 | -1 (0.55832) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15414 HOMO: -5.43411 LUMO: 0.45987 factor:1 | -1 (0.29484) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17630 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (1.27268) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30713 HOMO: -5.33071 LUMO: 1.14016 factor:1 | -1 (1.14184) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (1.35295) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59963 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-1.15066) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55958 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.11061) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26534 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.81637) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26042 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.81144) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53433 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.08535) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12108 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.67211) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01480 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.56582) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30327 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.85430) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58071 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-2.13174) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71520 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.26623) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45557 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-2.00659) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62595 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.17697) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12089 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.67192) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37762 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.92864) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55541 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.10644) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80328 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.35431) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07941 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.63043) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53141 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.08244) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31140 HOMO: -7.37429 LUMO: -0.08980 factor:1 | -1 (1.13757) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45377 HOMO: -7.28449 LUMO: -0.26395 factor:1 | -1 (0.99520) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64411 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-0.19513) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61651 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.16754) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30619 HOMO: -6.96611 LUMO: -0.30477 factor:1 | -1 (0.14278) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02047 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.57149) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -6.78924 LUMO: -0.73743 factor:1 | -1 (0.13429) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92964 HOMO: -7.57293 LUMO: -1.11295 factor:1 | -1 (0.51933) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02213 HOMO: -7.15932 LUMO: -0.23130 factor:1 | -1 (0.42684) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86915 HOMO: -7.48585 LUMO: -0.10068 factor:1 | -1 (0.57982) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16127 HOMO: -7.17020 LUMO: -0.26123 factor:1 | -1 (0.28771) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95778 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (0.49119) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16768 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-0.71871) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91094 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.46197) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11829 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.66932) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18912 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.74015) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73189 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-0.28292) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15613 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.70716) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45525 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.00628) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41585 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-0.96687) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19412 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.74515) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47027 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.02130) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17519 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.72622) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70619 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.25722) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82285 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.37388) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11225 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.66328) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79945 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.35048) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13816 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.68918) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02812 HOMO: -7.28721 LUMO: -0.18504 factor:1 | -1 (0.42085) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44533 HOMO: -7.49674 LUMO: -0.19864 factor:1 | -1 (0.00365) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50927 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-0.06030) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20286 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.75389) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40782 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-0.95885) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30080 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-0.85183) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77199 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.32302) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19892 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.74995) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08455 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.63558) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32725 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-0.87827) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30599 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.85702) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08654 HOMO: -6.75387 LUMO: -1.88031 factor:1 | -1 (0.36243) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75114 HOMO: -7.07768 LUMO: -1.25717 factor:1 | -1 (0.69784) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.91380 HOMO: -6.46543 LUMO: -1.14016 factor:1 | -1 (2.53518) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.73709 HOMO: -7.37973 LUMO: -0.45987 factor:1 | -1 (2.71189) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05096 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (1.39801) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89426 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.44529) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39743 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.94845) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52810 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.07913) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14510 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (0.30387) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83773 HOMO: -7.38245 LUMO: 0.10885 factor:1 | -1 (1.61124) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84938 HOMO: -7.59470 LUMO: -1.21363 factor:1 | -1 (1.59959) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00029 HOMO: -7.23279 LUMO: -1.23812 factor:1 | -1 (1.44868) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03232 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (1.41665) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93365 HOMO: -7.36340 LUMO: -0.17143 factor:1 | -1 (1.51532) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17992 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.73095) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.72575) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07105 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-0.62208) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34657 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-0.89759) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68304 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.23407) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50203 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-0.05306) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42935 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (0.01962) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15614 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-0.70717) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12093 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.67196) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42421 HOMO: -7.16204 LUMO: -0.23674 factor:1 | -1 (0.02476) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00964 HOMO: -6.81645 LUMO: -0.19320 factor:1 | -1 (0.43933) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23052 HOMO: -6.69400 LUMO: 0.04082 factor:1 | -1 (0.21845) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74264 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.29367) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28520 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (1.16378) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26057 HOMO: -6.60148 LUMO: -1.13744 factor:1 | -1 (1.18840) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28566 HOMO: -6.78108 LUMO: -0.82450 factor:1 | -1 (1.16331) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26922 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (1.17975) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24781 HOMO: -6.65318 LUMO: -1.26261 factor:1 | -1 (1.20117) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94788 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (1.50109) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23747 HOMO: -7.11850 LUMO: -0.99594 factor:1 | -1 (1.21151) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14846 HOMO: -6.64230 LUMO: -0.93879 factor:1 | -1 (1.30051) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01651 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (1.43246) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51710 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.06813) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37163 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-0.92266) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70106 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.25209) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33434 HOMO: -7.03142 LUMO: -0.35103 factor:1 | -1 (1.11463) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34398 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.89501) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59133 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-1.14236) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32568 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (0.12329) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33745 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.88848) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23620 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.78723) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22873 HOMO: -6.67495 LUMO: -0.96600 factor:1 | -1 (1.22024) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32424 HOMO: -6.74026 LUMO: -1.79867 factor:1 | -1 (1.12473) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77817 HOMO: -6.73482 LUMO: -1.78235 factor:1 | -1 (1.67081) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77632 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (1.67266) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10870 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (1.34027) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84336 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (1.60561) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03218 HOMO: -6.56883 LUMO: 0.22041 factor:1 | -1 (1.41679) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98078 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (1.46819) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04082 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.59185) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10325 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (0.34572) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12695 HOMO: -7.13483 LUMO: 0.33198 factor:1 | -1 (0.32202) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01614 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.56717) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13985 HOMO: -7.38517 LUMO: 0.17143 factor:1 | -1 (0.30912) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83495 HOMO: -6.80013 LUMO: 0.25851 factor:1 | -1 (0.61402) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79589 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-0.34692) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01647 HOMO: -6.51713 LUMO: -1.14560 factor:1 | -1 (0.43250) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99682 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.54785) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23686 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.21211) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99005 HOMO: -6.76475 LUMO: -0.16327 factor:1 | -1 (0.45892) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37114 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.92217) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49120 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-1.04222) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19742 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-0.74845) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13241 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-0.68344) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24104 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-0.79207) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11433 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.33465) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99100 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-0.54202) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-0.86812) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41432 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-0.96535) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78170 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (1.66727) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29287 HOMO: -6.68040 LUMO: -0.92247 factor:1 | -1 (1.15610) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88127 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (1.56770) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61446 HOMO: -6.94979 LUMO: -0.19864 factor:1 | -1 (1.83451) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21808 HOMO: -6.80829 LUMO: -0.30477 factor:1 | -1 (0.23089) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96970 HOMO: -7.22734 LUMO: -1.02859 factor:1 | -1 (0.47927) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05628 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.39269) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05032 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.60134) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12039 HOMO: -7.29809 LUMO: -0.97145 factor:1 | -1 (0.32858) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67894 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.22996) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76166 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.31269) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78452 HOMO: -7.36068 LUMO: -0.28028 factor:1 | -1 (0.66445) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03495 HOMO: -7.10761 LUMO: -1.14832 factor:1 | -1 (0.41402) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96207 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.51310) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10377 HOMO: -6.91713 LUMO: -1.81228 factor:1 | -1 (0.34520) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22987 HOMO: -6.78652 LUMO: -2.01636 factor:1 | -1 (1.21910) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08002 HOMO: -6.52801 LUMO: -1.17553 factor:1 | -1 (1.36895) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05469 HOMO: -7.54844 LUMO: -1.18642 factor:1 | -1 (1.39428) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90470 HOMO: -7.52939 LUMO: -1.23812 factor:1 | -1 (1.54427) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.64758 HOMO: -7.94572 LUMO: -0.81634 factor:1 | -1 (1.80139) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27477 HOMO: -7.55932 LUMO: -0.86260 factor:1 | -1 (1.17420) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37701 HOMO: -7.72259 LUMO: -1.39050 factor:1 | -1 (1.07197) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86753 HOMO: -7.11850 LUMO: -1.01498 factor:1 | -1 (1.58144) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.14975 HOMO: -7.09673 LUMO: -1.00954 factor:1 | -1 (2.29923) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48871 HOMO: -6.06270 LUMO: 0.16327 factor:1 | -1 (0.96026) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36201 HOMO: -5.71167 LUMO: 0.70477 factor:1 | -1 (1.08696) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98973 HOMO: -5.38241 LUMO: 0.86260 factor:1 | -1 (1.45924) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93664 HOMO: -5.67357 LUMO: 1.27621 factor:1 | -1 (0.51234) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15039 HOMO: -7.56204 LUMO: -0.68573 factor:1 | -1 (1.29858) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -5.57833 LUMO: 1.13199 factor:1 | -1 (1.12516) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22547 HOMO: -7.58653 LUMO: -0.66124 factor:1 | -1 (1.22351) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34517 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (1.10380) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37837 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (1.07060) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52743 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (0.92154) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -6.63686 LUMO: 0.09252 factor:1 | -1 (0.47748) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15378 HOMO: -6.84366 LUMO: -0.14422 factor:1 | -1 (0.29519) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84610 HOMO: -6.93074 LUMO: 0.04354 factor:1 | -1 (0.60287) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25457 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (0.19440) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95887 HOMO: -6.59876 LUMO: -0.10068 factor:1 | -1 (0.49010) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30310 HOMO: -6.74570 LUMO: -0.44627 factor:1 | -1 (1.14587) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27790 HOMO: -6.60148 LUMO: -0.61770 factor:1 | -1 (1.17107) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97364 HOMO: -6.55794 LUMO: -1.06941 factor:1 | -1 (0.47533) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92904 HOMO: -7.12666 LUMO: -0.11973 factor:1 | -1 (0.51993) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25898 HOMO: -7.21646 LUMO: -0.50069 factor:1 | -1 (0.18999) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91391 HOMO: -7.27632 LUMO: -1.00682 factor:1 | -1 (0.53506) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63083 HOMO: -6.74298 LUMO: 0.04354 factor:1 | -1 (0.81814) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00820 HOMO: -6.37291 LUMO: 0.14150 factor:1 | -1 (0.44077) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40691 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (1.04206) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32838 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (1.12059) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20593 HOMO: -6.51985 LUMO: -0.10885 factor:1 | -1 (1.24304) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35733 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (1.09164) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05678 HOMO: -5.58922 LUMO: 0.24490 factor:1 | -1 (1.39219) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31091 HOMO: -6.32665 LUMO: -0.57144 factor:1 | -1 (1.13806) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24103 HOMO: -6.29127 LUMO: -0.93607 factor:1 | -1 (1.20794) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87025 HOMO: -5.49670 LUMO: 0.27211 factor:1 | -1 (1.57872) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12326 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (1.32571) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70961 HOMO: -5.68174 LUMO: 0.69933 factor:1 | -1 (0.73936) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45182 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-1.00285) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44951 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.00054) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36298 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.91400) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56140 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.11243) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31182 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.86285) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24934 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-0.80037) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43468 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.98571) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01731 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.56834) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02351 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-0.57454) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48692 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.03795) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99589 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-0.54692) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45705 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.00807) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71385 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.26488) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22229 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-0.77332) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32809 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.87912) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35272 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-0.90374) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38994 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.94097) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53755 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-0.08857) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43038 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.98141) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.67661) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (0.47748) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78037 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (1.66860) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31753 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.86856) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20474 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.75577) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94087 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.49190) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44445 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.99547) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50320 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-1.05422) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11408 HOMO: -5.60555 LUMO: 0.67484 factor:1 | -1 (0.33489) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27435 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.82538) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01315 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.56417) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67087 HOMO: -5.82868 LUMO: 0.91974 factor:1 | -1 (1.77810) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.72987 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (1.71911) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.53827 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (1.91070) | -1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04149 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (1.40748) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88181 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (1.56716) | 1 | -1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98027 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-0.53130) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98447 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (0.46450) | 1 | 1 |
| G: -5717.08328 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79089 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (0.65808) | 1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91518 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-0.46621) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01816 HOMO: -7.35524 LUMO: -1.25444 factor:1 | -1 (0.43081) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66499 HOMO: -6.81645 LUMO: -1.20819 factor:1 | -1 (0.78399) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66623 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.21726) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71750 HOMO: -6.88992 LUMO: -0.47620 factor:1 | -1 (0.73147) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42743 HOMO: -7.22190 LUMO: -0.01905 factor:1 | -1 (1.02154) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85928 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (1.58969) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19028 HOMO: -6.48447 LUMO: -0.95512 factor:1 | -1 (1.25869) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97352 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (1.47546) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90845 HOMO: -7.36612 LUMO: 0.19320 factor:1 | -1 (1.54052) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10263 HOMO: -7.24095 LUMO: 0.33470 factor:1 | -1 (1.34634) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15379 HOMO: -7.15932 LUMO: -2.24222 factor:1 | -1 (1.29518) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31194 HOMO: -6.88992 LUMO: -2.69937 factor:1 | -1 (1.13703) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68087 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.23190) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39354 HOMO: -7.17564 LUMO: -0.93879 factor:1 | -1 (0.05543) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91663 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.46765) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00008 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.55111) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00077 HOMO: -7.17292 LUMO: -1.07213 factor:1 | -1 (0.44820) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01283 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.43614) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06585 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-1.61687) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37936 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.93038) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02944 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-1.58046) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25503 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.80606) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39333 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.94436) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12232 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.67335) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64478 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-1.19580) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75346 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-1.30449) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06194 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.61296) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79706 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.34809) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71747 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-0.26849) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61591 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.16694) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84937 HOMO: -6.55794 LUMO: -0.84900 factor:1 | -1 (0.59960) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.26923 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (2.17974) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.96710 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (2.48187) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01897 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (2.43000) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89972 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (1.54925) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88905 HOMO: -6.74298 LUMO: -0.85172 factor:1 | -1 (1.55992) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70486 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (1.74411) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77242 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (1.67655) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.65275 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (1.79622) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95175 HOMO: -7.09129 LUMO: -0.85988 factor:1 | -1 (1.49722) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04530 HOMO: -6.57971 LUMO: -2.27215 factor:1 | -1 (1.40367) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92524 HOMO: -6.81373 LUMO: -1.86942 factor:1 | -1 (1.52373) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16481 HOMO: -6.59060 LUMO: -2.30480 factor:1 | -1 (1.28416) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65252 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.79645) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70279 HOMO: -6.94707 LUMO: -2.62318 factor:1 | -1 (1.74618) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.75961 HOMO: -7.28177 LUMO: -0.09796 factor:1 | -1 (1.68936) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67729 HOMO: -6.80013 LUMO: -0.79729 factor:1 | -1 (1.77168) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.33416 HOMO: -7.26544 LUMO: 0.12789 factor:1 | -1 (2.11481) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40662 HOMO: -6.51713 LUMO: -0.49253 factor:1 | -1 (2.04235) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43777 HOMO: -6.68856 LUMO: -0.77280 factor:1 | -1 (1.01120) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.03478 HOMO: -6.41100 LUMO: -0.70750 factor:1 | -1 (2.41419) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.31990 HOMO: -7.56204 LUMO: 0.22041 factor:1 | -1 (2.12907) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01309 HOMO: -6.68312 LUMO: 1.30343 factor:1 | -1 (2.43588) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.06150 HOMO: -7.24367 LUMO: 0.17415 factor:1 | -1 (2.38747) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.80016 HOMO: -7.52395 LUMO: 1.16737 factor:1 | -1 (2.64881) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.86735 HOMO: -6.89264 LUMO: 0.23130 factor:1 | -1 (2.58163) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.85516 HOMO: -7.21102 LUMO: 0.19048 factor:1 | -1 (2.59382) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38182 HOMO: -7.08312 LUMO: 0.25034 factor:1 | -1 (1.06715) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26658 HOMO: -6.49536 LUMO: -0.65852 factor:1 | -1 (1.18239) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24261 HOMO: -6.85455 LUMO: 0.13606 factor:1 | -1 (1.20636) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44025 HOMO: -7.10217 LUMO: 0.35919 factor:1 | -1 (1.00873) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19684 HOMO: -7.77429 LUMO: 1.19186 factor:1 | -1 (1.25213) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07523 HOMO: -6.57427 LUMO: -0.50069 factor:1 | -1 (1.37374) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -7.36340 LUMO: 0.10068 factor:1 | -1 (1.28070) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96650 HOMO: -7.28177 LUMO: 0.15238 factor:1 | -1 (1.48248) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74962 HOMO: -6.86543 LUMO: -0.84355 factor:1 | -1 (1.69935) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73392 HOMO: -6.55794 LUMO: 1.39594 factor:1 | -1 (1.71505) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.43971 HOMO: -6.26134 LUMO: 1.53744 factor:1 | -1 (2.00926) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84878 HOMO: -5.97562 LUMO: 1.42316 factor:1 | -1 (1.60019) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88611 HOMO: -6.65046 LUMO: 1.44492 factor:1 | -1 (1.56286) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75073 HOMO: -6.92258 LUMO: 0.17415 factor:1 | -1 (0.69824) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43265 HOMO: -7.40966 LUMO: 0.19592 factor:1 | -1 (1.01632) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89397 HOMO: -7.17564 LUMO: 0.16871 factor:1 | -1 (0.55500) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88548 HOMO: -7.46953 LUMO: 0.22313 factor:1 | -1 (0.56349) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84210 HOMO: -6.13345 LUMO: 1.85854 factor:1 | -1 (0.60687) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20570 HOMO: -6.99333 LUMO: -1.65717 factor:1 | -1 (0.24327) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64343 HOMO: -6.93074 LUMO: -1.79323 factor:1 | -1 (0.80554) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49666 HOMO: -6.87904 LUMO: -1.79323 factor:1 | -1 (1.95231) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.39887 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (2.05011) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03648 HOMO: -7.13210 LUMO: -1.17553 factor:1 | -1 (1.41249) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15679 HOMO: -6.52801 LUMO: -2.23678 factor:1 | -1 (1.29219) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43635 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (1.01262) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52548 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-1.07651) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29761 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.84864) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02011 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.57114) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08825 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.63928) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39873 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.94976) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82871 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.37973) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51699 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.06802) | 1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96196 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.51299) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55297 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.10399) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32850 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.87953) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75031 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.30134) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37098 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.92200) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10224 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.65326) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81483 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.36586) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52693 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-0.07796) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28066 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-0.83169) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33770 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.88872) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43088 HOMO: -6.93890 LUMO: -2.65039 factor:1 | -1 (0.01810) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35941 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.91044) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00525 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-1.55627) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96418 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-1.51521) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32714 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.87817) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08693 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.63796) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51486 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-2.06589) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41680 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.96783) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71754 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.26857) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53263 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-2.08366) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10830 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.65933) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.72575) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85550 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.40653) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46603 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.01705) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68269 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.23372) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61436 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.16539) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66895 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.21998) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50654 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.05757) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25142 HOMO: -7.27088 LUMO: -1.18642 factor:1 | -1 (0.19755) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45675 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.00777) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51364 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.06467) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13080 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.68183) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40047 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.95150) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11896 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.66999) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47748 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.02851) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18351 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.73454) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.46452 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-2.01555) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64412 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.19515) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07777 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.62880) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93493 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.48596) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45544 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.00647) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76845 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.31948) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34209 HOMO: -7.00965 LUMO: -1.37690 factor:1 | -1 (1.10688) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14998 HOMO: -6.97972 LUMO: -1.58098 factor:1 | -1 (1.29899) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27535 HOMO: -6.91169 LUMO: -1.48574 factor:1 | -1 (1.17363) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04841 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.59944) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.78652 LUMO: -1.51840 factor:1 | -1 (0.34210) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78099 HOMO: -6.84638 LUMO: -1.15104 factor:1 | -1 (0.66799) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78872 HOMO: -6.61237 LUMO: -0.89798 factor:1 | -1 (0.66026) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06184 HOMO: -7.16204 LUMO: -1.30070 factor:1 | -1 (0.38714) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82300 HOMO: -7.32803 LUMO: 0.14694 factor:1 | -1 (0.62597) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92940 HOMO: -6.99877 LUMO: -0.87621 factor:1 | -1 (0.51957) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67475 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (0.77422) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03318 HOMO: -7.08040 LUMO: -1.09662 factor:1 | -1 (0.41579) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61367 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-1.16470) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24468 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-1.79571) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64848 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-1.19951) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51290 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-2.06393) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06775 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.61878) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86095 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.41198) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79950 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.35053) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83267 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.38370) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18322 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.73424) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54146 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.09249) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.81732) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12188 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.67291) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39895 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.94998) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52001 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.07104) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90072 HOMO: -6.78380 LUMO: 1.81500 factor:1 | -1 (0.54826) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10628 HOMO: -6.49536 LUMO: 1.70615 factor:1 | -1 (1.34269) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19304 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.74407) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94844 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-0.49946) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31106 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.86208) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.68772 HOMO: -6.18243 LUMO: 1.77962 factor:1 | -1 (1.76126) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30307 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (1.14590) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89962 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-0.45065) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23607 HOMO: -6.84094 LUMO: -0.84900 factor:1 | -1 (0.21290) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12532 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (0.32365) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79687 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.34790) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61635 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.16738) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37547 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.92649) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04887 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.59990) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64721 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.19823) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83146 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.38248) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01462 HOMO: -7.39061 LUMO: 0.17687 factor:1 | -1 (0.43435) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71372 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (0.73525) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99007 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.54110) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15313 HOMO: -7.33347 LUMO: 0.33198 factor:1 | -1 (0.29584) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91930 HOMO: -7.31986 LUMO: -0.83539 factor:1 | -1 (0.52967) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46018 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.01121) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00413 HOMO: -7.36884 LUMO: 0.38096 factor:1 | -1 (1.44484) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24869 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-0.79972) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57152 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.12255) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53686 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.08788) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60246 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.15349) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30465 HOMO: -6.57699 LUMO: 1.81228 factor:1 | -1 (1.14432) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15445 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-0.70548) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27216 HOMO: -6.91169 LUMO: -1.22451 factor:1 | -1 (1.17681) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32196 HOMO: -7.09945 LUMO: -1.23812 factor:1 | -1 (1.12701) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96241 HOMO: -7.48857 LUMO: 0.10340 factor:1 | -1 (1.48656) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22947 HOMO: -7.21918 LUMO: -0.06803 factor:1 | -1 (1.21951) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03894 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.58997) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09729 HOMO: -6.82734 LUMO: -0.77825 factor:1 | -1 (0.35168) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16352 HOMO: -6.92258 LUMO: -1.03675 factor:1 | -1 (0.28545) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73205 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.28308) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89405 HOMO: -6.96067 LUMO: -1.05036 factor:1 | -1 (0.55492) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30859 HOMO: -7.23551 LUMO: 0.12245 factor:1 | -1 (0.14038) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39118 HOMO: -6.85183 LUMO: 0.16055 factor:1 | -1 (0.05780) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10927 HOMO: -6.46815 LUMO: -0.89253 factor:1 | -1 (0.33971) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12770 HOMO: -7.23823 LUMO: -0.06259 factor:1 | -1 (1.32128) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36756 HOMO: -6.76475 LUMO: -0.99049 factor:1 | -1 (1.08141) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30612 HOMO: -7.14843 LUMO: -0.88165 factor:1 | -1 (1.14285) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43853 HOMO: -7.15659 LUMO: 0.20681 factor:1 | -1 (1.01044) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84012 HOMO: -7.11306 LUMO: 0.14150 factor:1 | -1 (0.60885) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40884 HOMO: -6.67223 LUMO: -0.86260 factor:1 | -1 (0.04014) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88765 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.43867) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79105 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.34207) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16259 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.71362) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45735 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.00838) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97929 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.53032) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28172 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.83275) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29267 HOMO: -7.05047 LUMO: -1.06669 factor:1 | -1 (0.15630) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83728 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.38831) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19108 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-0.74211) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83099 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-0.38202) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12200 HOMO: -6.68856 LUMO: 1.61364 factor:1 | -1 (0.32697) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86366 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (0.58532) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28051 HOMO: -6.73482 LUMO: 1.86398 factor:1 | -1 (0.16847) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99672 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (0.45225) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72675 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-0.27777) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39093 HOMO: -6.35114 LUMO: 1.71432 factor:1 | -1 (0.05804) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18149 HOMO: -6.34842 LUMO: 1.92929 factor:1 | -1 (1.26748) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20253 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (1.24644) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29875 HOMO: -6.31032 LUMO: 1.51567 factor:1 | -1 (1.15023) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17221 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (1.27676) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22664 HOMO: -6.49264 LUMO: 1.66806 factor:1 | -1 (1.22234) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87526 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (1.57372) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88903 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (1.55995) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13600 HOMO: -7.35252 LUMO: 0.03537 factor:1 | -1 (1.31298) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73778 HOMO: -6.58243 LUMO: -0.48980 factor:1 | -1 (1.71119) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12683 HOMO: -6.90081 LUMO: -0.05442 factor:1 | -1 (1.32215) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04203 HOMO: -7.22734 LUMO: 0.17143 factor:1 | -1 (1.40694) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46984 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.02087) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95253 HOMO: -7.39878 LUMO: 0.13334 factor:1 | -1 (0.49644) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09331 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.64434) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70483 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.25586) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32668 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.87770) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40902 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.96004) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14711 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-0.69814) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96074 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.51176) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93230 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.48333) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12300 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.67403) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15949 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-0.71052) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74698 HOMO: -7.09401 LUMO: 0.04354 factor:1 | -1 (1.70199) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11374 HOMO: -6.85183 LUMO: -0.68573 factor:1 | -1 (1.33524) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89542 HOMO: -6.83006 LUMO: -0.58777 factor:1 | -1 (1.55355) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94317 HOMO: -7.40422 LUMO: 0.17687 factor:1 | -1 (0.50581) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57146 HOMO: -7.15932 LUMO: 0.10340 factor:1 | -1 (0.87751) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69875 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.24977) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04055 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-0.59158) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10399 HOMO: -7.49402 LUMO: 0.11429 factor:1 | -1 (0.34499) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37006 HOMO: -7.01237 LUMO: -1.06397 factor:1 | -1 (0.07891) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64827 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.19930) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81274 HOMO: -7.38789 LUMO: -1.15376 factor:1 | -1 (0.63623) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66275 HOMO: -6.42461 LUMO: -1.23812 factor:1 | -1 (0.78622) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80773 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-0.35875) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.65591 LUMO: 0.07075 factor:1 | -1 (0.52741) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76295 HOMO: -7.39061 LUMO: -0.16871 factor:1 | -1 (0.68603) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10423 HOMO: -6.90353 LUMO: -0.96056 factor:1 | -1 (0.34474) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98827 HOMO: -7.42054 LUMO: 0.19048 factor:1 | -1 (1.46071) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50585 HOMO: -7.40150 LUMO: 0.35647 factor:1 | -1 (0.94312) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35295 HOMO: -6.56067 LUMO: -0.96056 factor:1 | -1 (1.09602) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23926 HOMO: -6.89809 LUMO: -0.81090 factor:1 | -1 (1.20971) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85400 HOMO: -6.91986 LUMO: -0.84900 factor:1 | -1 (1.59497) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04895 HOMO: -6.61509 LUMO: -0.62042 factor:1 | -1 (1.40003) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07540 HOMO: -6.58243 LUMO: -0.65579 factor:1 | -1 (1.37358) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12315 HOMO: -6.52257 LUMO: -0.92519 factor:1 | -1 (1.32582) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32751 HOMO: -6.69128 LUMO: 1.49118 factor:1 | -1 (1.12146) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25374 HOMO: -7.02870 LUMO: 1.67894 factor:1 | -1 (1.19523) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28196 HOMO: -6.88720 LUMO: 1.68711 factor:1 | -1 (1.16701) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96933 HOMO: -5.89943 LUMO: 1.03675 factor:1 | -1 (1.47965) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01798 HOMO: -6.40556 LUMO: 1.14560 factor:1 | -1 (1.43099) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61593 HOMO: -6.51168 LUMO: 1.48030 factor:1 | -1 (1.83304) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86053 HOMO: -6.64502 LUMO: 1.91568 factor:1 | -1 (1.58844) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37486 HOMO: -6.47903 LUMO: 1.91296 factor:1 | -1 (1.07412) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33045 HOMO: -6.34297 LUMO: 1.91840 factor:1 | -1 (1.11852) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20933 HOMO: -6.89809 LUMO: 1.82861 factor:1 | -1 (1.23964) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36833 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (1.08065) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88965 HOMO: -7.16476 LUMO: -0.92247 factor:1 | -1 (1.55932) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88761 HOMO: -7.10489 LUMO: -0.95784 factor:1 | -1 (1.56136) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22250 HOMO: -6.76475 LUMO: -0.99866 factor:1 | -1 (1.22647) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04984 HOMO: -6.81373 LUMO: -1.05036 factor:1 | -1 (1.39913) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79949 HOMO: -6.90081 LUMO: -1.03947 factor:1 | -1 (0.64948) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64286 HOMO: -7.06952 LUMO: -0.91702 factor:1 | -1 (0.80611) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85389 HOMO: -6.73482 LUMO: -0.94151 factor:1 | -1 (0.59509) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64202 HOMO: -6.99605 LUMO: -1.04764 factor:1 | -1 (0.80695) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29847 HOMO: -7.03686 LUMO: -0.93335 factor:1 | -1 (1.15050) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33431 HOMO: -6.81101 LUMO: -0.95240 factor:1 | -1 (1.11466) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44295 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-0.99398) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44409 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.99512) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41664 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.96766) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17894 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.72997) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13870 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-0.68973) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19704 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-0.74807) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23413 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.78516) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09312 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.64415) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14120 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.69223) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15372 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-0.70475) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01472 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.56575) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95388 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.50491) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16817 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.71920) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84536 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-0.39639) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02536 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95534 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.50637) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19416 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.74518) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01357 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-1.56460) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.86910) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85115 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.40218) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34923 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.90025) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.73800) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97077 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-1.52180) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81890 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-1.36993) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09617 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.64720) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89071 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.44174) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27739 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.82841) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06909 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.62012) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25048 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.80151) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63795 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.18897) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92542 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-0.47644) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75691 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.30794) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13312 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.68415) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18501 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.73604) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95246 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-1.50348) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21522 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-0.76625) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00406 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.55509) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20422 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.75525) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11782 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-1.66885) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11447 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.66550) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71066 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.26168) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82601 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-0.37704) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27710 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-0.82812) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12118 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-0.67220) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23870 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-0.78973) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29462 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.84565) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91929 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.47032) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43465 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.98568) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62336 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.17439) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41106 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.96209) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.89667) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24931 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.80034) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06273 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (0.38624) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30011 HOMO: -7.22462 LUMO: -1.18642 factor:1 | -1 (1.14886) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00437 HOMO: -7.18381 LUMO: -0.78641 factor:1 | -1 (1.44460) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92628 HOMO: -6.93346 LUMO: 1.65717 factor:1 | -1 (1.52269) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38899 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.94002) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32752 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.87855) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34643 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.89746) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23669 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.78772) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.86910) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27424 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.82527) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24341 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.79444) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12183 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.67286) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18048 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (0.26849) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24627 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.79729) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14206 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (1.30691) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89635 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (1.55263) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07017 HOMO: -5.95929 LUMO: 1.62724 factor:1 | -1 (1.37880) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93866 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (1.51031) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02765 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.57868) | 1 | 1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17846 HOMO: -6.90897 LUMO: 1.71432 factor:1 | -1 (0.27051) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88332 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.43435) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92929 HOMO: -6.83278 LUMO: 1.61908 factor:1 | -1 (0.51968) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93314 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.48417) | 1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13868 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.31029) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10633 HOMO: -6.53073 LUMO: 1.51023 factor:1 | -1 (0.34265) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15327 HOMO: -6.93346 LUMO: 2.22861 factor:1 | -1 (0.29571) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93362 HOMO: -6.47903 LUMO: 2.05446 factor:1 | -1 (0.51536) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94083 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (0.50815) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87751 HOMO: -6.07358 LUMO: 1.95922 factor:1 | -1 (0.57147) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62928 HOMO: -6.75114 LUMO: 2.18780 factor:1 | -1 (0.81969) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72455 HOMO: -6.96339 LUMO: 1.70071 factor:1 | -1 (0.72442) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06197 HOMO: -7.14843 LUMO: 1.82588 factor:1 | -1 (0.38700) | 1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94736 HOMO: -6.96339 LUMO: 2.29392 factor:1 | -1 (0.50161) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31001 HOMO: -6.81645 LUMO: 2.39732 factor:1 | -1 (1.13896) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88725 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (0.56172) | -1 | -1 |
| G: -5717.08328 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62879 HOMO: -7.14843 LUMO: 2.01092 factor:1 | -1 (0.82018) | 1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.51587 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (0.93311) | 1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94646 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (0.50251) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67459 HOMO: -7.07768 LUMO: -0.26123 factor:1 | -1 (0.77438) | 1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38153 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-0.93256) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34766 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.89868) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14534 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.69637) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83075 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.38178) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91597 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.46700) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75777 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.30879) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43705 HOMO: -7.08040 LUMO: -0.85716 factor:1 | -1 (0.01192) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64043 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.19146) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31644 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.86747) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43902 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.99005) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42134 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.97237) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.36065 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.91168) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71036 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.26138) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06795 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.61898) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81270 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-1.36373) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40431 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.95534) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48466 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.03569) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27701 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.82804) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79275 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.34378) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98422 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.53525) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89396 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.44499) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29993 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.85095) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05619 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-1.60721) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94277 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-1.49380) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13288 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-0.68390) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05783 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-0.60885) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40428 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-0.95531) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52498 HOMO: -6.77291 LUMO: -0.70477 factor:1 | -1 (0.92399) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91215 HOMO: -6.76475 LUMO: -1.15921 factor:1 | -1 (0.53683) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67048 HOMO: -5.37697 LUMO: -0.56600 factor:1 | -1 (0.77849) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80189 HOMO: -6.62053 LUMO: -1.75513 factor:1 | -1 (0.64709) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17753 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.72856) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29819 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.84921) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89869 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.44972) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65743 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.20846) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54678 HOMO: -7.02326 LUMO: 0.11429 factor:1 | -1 (0.90219) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62392 HOMO: -7.40966 LUMO: 0.18232 factor:1 | -1 (0.82505) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55810 HOMO: -6.34570 LUMO: 0.41089 factor:1 | -1 (0.89087) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47407 HOMO: -6.78924 LUMO: 0.49525 factor:1 | -1 (0.97490) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77650 HOMO: -6.87632 LUMO: 0.44082 factor:1 | -1 (0.67247) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93968 HOMO: -6.69944 LUMO: 1.20546 factor:1 | -1 (0.50929) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66654 HOMO: -6.83006 LUMO: 1.28982 factor:1 | -1 (0.78244) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89535 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.44638) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99301 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.54404) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71330 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-0.26433) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47012 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.02114) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81875 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.36978) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62794 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-0.17897) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12749 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.67852) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62929 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.18032) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87950 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.43053) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04044 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-0.59147) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19973 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.75075) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69615 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.24718) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48330 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.03433) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70192 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-1.25295) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92218 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.47321) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80871 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.35973) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11733 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-1.66836) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30499 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.85602) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16795 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.71898) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16705 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.71808) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82865 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.37968) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83575 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.38678) | 1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75709 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-0.30811) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66457 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.21560) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23963 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.79065) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33538 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-0.88641) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72185 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-0.27288) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58653 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.13755) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24578 HOMO: -6.68040 LUMO: 0.22041 factor:1 | -1 (0.20319) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30999 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.86102) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23432 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.78535) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04966 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.60069) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81448 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.36550) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92104 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.47206) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11881 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.66984) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81647 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (0.63250) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82593 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.37696) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87268 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.42371) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08328 HOMO: -7.33619 LUMO: 1.45581 factor:1 | -1 (0.36569) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87487 HOMO: -6.87904 LUMO: -0.14422 factor:1 | -1 (0.57411) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93530 HOMO: -6.81917 LUMO: 0.50341 factor:1 | -1 (0.51367) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06711 HOMO: -7.27905 LUMO: 0.13606 factor:1 | -1 (0.38186) | 1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11185 HOMO: -6.87904 LUMO: -0.09796 factor:1 | -1 (0.33712) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13852 HOMO: -7.33891 LUMO: 0.03810 factor:1 | -1 (0.31045) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89476 HOMO: -6.98516 LUMO: 0.98233 factor:1 | -1 (0.55421) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53935 HOMO: -6.94162 LUMO: 0.86804 factor:1 | -1 (0.90962) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18584 HOMO: -7.37701 LUMO: 0.05442 factor:1 | -1 (0.26313) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04333 HOMO: -7.04775 LUMO: 0.43266 factor:1 | -1 (0.40564) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58759 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.13861) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08218 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.63321) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95033 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-1.50136) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91867 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.46970) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91339 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.46442) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04755 HOMO: -6.85455 LUMO: 0.23946 factor:1 | -1 (0.40142) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82866 HOMO: -6.93346 LUMO: 0.24762 factor:1 | -1 (0.62031) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84061 HOMO: -6.85455 LUMO: 0.17687 factor:1 | -1 (0.60836) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79642 HOMO: -6.62325 LUMO: 0.69933 factor:1 | -1 (0.65256) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98058 HOMO: -6.43005 LUMO: 0.50069 factor:1 | -1 (0.46839) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83726 HOMO: -6.56883 LUMO: 0.22858 factor:1 | -1 (0.61171) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93446 HOMO: -6.78380 LUMO: 0.54967 factor:1 | -1 (0.51451) | -1 | -1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79791 HOMO: -7.35524 LUMO: 0.00272 factor:1 | -1 (0.65106) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09565 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.64668) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24893 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.79996) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82480 HOMO: -7.27360 LUMO: 0.29933 factor:1 | -1 (0.62417) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85176 HOMO: -7.09129 LUMO: 0.41089 factor:1 | -1 (0.59721) | 1 | 1 |
| G: -5717.08328 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86041 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.41144) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38572 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.93675) | -1 | -1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43532 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-1.98635) | -1 | -1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51614 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-2.06717) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69196 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-1.24299) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50896 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-2.05998) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23997 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-1.79100) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42613 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.97716) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43997 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.00901) | -1 | -1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39789 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.94892) | 1 | 1 |
| G: -5717.08328 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42885 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.97988) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46886 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.01989) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55646 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.10748) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28031 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.83134) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24093 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.79196) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13765 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.31133) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71926 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.27029) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36701 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.08196) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45394 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.00497) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23873 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.78976) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41330 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.03567) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51681 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.06784) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90544 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.45647) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12256 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.67359) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30967 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.86070) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13261 HOMO: -6.50896 LUMO: -0.43810 factor:1 | -1 (0.31636) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75584 HOMO: -6.73210 LUMO: -0.51430 factor:1 | -1 (0.69313) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07593 HOMO: -6.77019 LUMO: -0.62858 factor:1 | -1 (0.37304) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35063 HOMO: -6.82462 LUMO: -0.67484 factor:1 | -1 (0.09834) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26316 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.81419) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12738 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.67841) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51572 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.06675) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32255 HOMO: -6.49536 LUMO: -0.25307 factor:1 | -1 (0.12642) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13239 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.68341) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61596 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.16699) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70013 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.25116) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06901 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.62004) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29916 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.85018) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61767 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-2.16869) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.76131 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-2.31234) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19496 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.74599) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.57807 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-2.12910) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78505 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.33608) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20216 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.75318) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64023 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.19126) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43518 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.01380) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60669 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.15772) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04060 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.59163) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76773 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.31875) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63653 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.18756) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84411 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.39514) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91277 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.53620) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84066 HOMO: -6.23957 LUMO: 1.78507 factor:1 | -1 (0.60831) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70384 HOMO: -6.35114 LUMO: 1.92112 factor:1 | -1 (0.74513) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92022 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.47125) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27278 HOMO: -6.60420 LUMO: 1.78779 factor:1 | -1 (0.17619) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23365 HOMO: -7.40422 LUMO: -0.97145 factor:1 | -1 (0.21532) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04918 HOMO: -6.80013 LUMO: -0.69117 factor:1 | -1 (0.39979) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05527 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.60630) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95442 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.50544) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25574 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.80676) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32465 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.87568) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.77629) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11137 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.66240) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18432 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.73535) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41816 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.96919) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44475 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.99577) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06760 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (0.38137) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97875 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.52978) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93067 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.48170) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87943 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.43046) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06319 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.61422) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97415 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.52518) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96030 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.51133) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93973 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.49076) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94251 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.49353) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87385 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.42488) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15794 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.70897) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90748 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.45851) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70090 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.25192) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74830 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.29933) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43980 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.00917) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70606 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.25708) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97647 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.52749) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85107 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.40210) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99660 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.54763) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98106 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.53209) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70753 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.25856) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82833 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.37935) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69235 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.24338) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50174 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.05276) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95377 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.50480) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07840 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.62943) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10896 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.65998) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23543 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.78645) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17415 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.72517) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35669 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.90772) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91734 HOMO: -6.85727 LUMO: 1.99187 factor:1 | -1 (0.53163) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65244 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.79653) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48327 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.96570) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80262 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.64635) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73405 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.71492) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62318 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.17421) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99320 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.54423) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75717 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.30820) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52677 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.07780) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68903 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.24006) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87611 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.42714) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94435 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.49537) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99198 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.54300) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73542 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.28645) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80482 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.35584) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50067 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.05170) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67616 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.22719) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43022 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.01875) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89235 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.44338) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83535 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.38637) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33887 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.88989) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62927 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.18030) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22188 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.77291) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49597 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.04699) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23476 HOMO: -6.66135 LUMO: 1.92384 factor:1 | -1 (0.21421) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33569 HOMO: -6.64502 LUMO: 2.15786 factor:1 | -1 (0.11328) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96885 HOMO: -6.71305 LUMO: 1.91840 factor:1 | -1 (0.48012) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94786 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (1.50112) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84859 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (1.60038) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07970 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (1.36928) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94073 HOMO: -6.60420 LUMO: -0.22585 factor:1 | -1 (1.50825) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12681 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.67784) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34235 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.89338) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93399 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.48502) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27051 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.82154) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60753 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.15856) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48206 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.03309) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40026 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.95128) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42635 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.97738) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76890 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.31992) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19391 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.74494) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23840 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.78943) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58457 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.13559) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04667 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.59770) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37286 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.07611) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22900 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.21998) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02003 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.57106) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89954 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.45057) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47822 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.02925) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41609 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.96712) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.89667) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28912 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.84015) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32300 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.87403) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15323 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.70426) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -6.66407 LUMO: 1.95650 factor:1 | -1 (0.24539) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21916 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.77019) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43664 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.98766) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88786 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (1.56112) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87643 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (1.57255) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94127 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (1.50770) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06097 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (1.38800) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33507 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.11391) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92420 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (0.52477) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66986 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (0.77912) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04347 HOMO: -6.01372 LUMO: 2.01636 factor:1 | -1 (0.40550) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70596 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.25698) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85615 HOMO: -6.53073 LUMO: 2.20684 factor:1 | -1 (0.59283) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87484 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.57413) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86171 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.41274) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05041 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (0.39857) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94417 HOMO: -6.88992 LUMO: 1.65173 factor:1 | -1 (0.50480) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94894 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.50004) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.41781 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (2.03117) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08514 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (1.36383) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31053 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (1.13844) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92854 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (1.52044) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03148 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (1.41750) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13034 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (1.31864) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29292 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (1.15605) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71666 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.73231) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94420 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (0.50477) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89025 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (1.55872) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88315 HOMO: -7.08584 LUMO: 1.99187 factor:1 | -1 (1.56582) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87594 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (1.57304) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09684 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (1.35213) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10400 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (1.34498) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34817 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.89920) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97429 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.52532) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41294 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.96396) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31010 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.86113) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04490 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.59593) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27663 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.82766) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05464 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.60567) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76247 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.31350) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17280 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.72382) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83427 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.61471) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46149 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.01252) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77696 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (0.67201) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21531 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (0.23366) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56349 HOMO: -6.56611 LUMO: -0.77008 factor:1 | -1 (0.88549) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38219 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.93321) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33944 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.89047) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74770 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.29873) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.81732) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26284 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.81387) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67806 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.22909) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26758 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (0.18139) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04477 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.59579) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44639 HOMO: -6.65046 LUMO: -0.41361 factor:1 | -1 (0.00259) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99081 HOMO: -6.76475 LUMO: -0.60137 factor:1 | -1 (0.45816) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69686 HOMO: -6.77836 LUMO: -0.54423 factor:1 | -1 (1.75211) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.91626 HOMO: -7.52395 LUMO: 0.26395 factor:1 | -1 (1.53271) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98176 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (1.46721) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.04270 HOMO: -6.72938 LUMO: -0.47348 factor:1 | -1 (2.40628) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29195 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (2.15702) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.25568 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (2.19329) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05821 HOMO: -6.67495 LUMO: -0.27211 factor:1 | -1 (2.39077) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12024 HOMO: -7.23823 LUMO: -0.62858 factor:1 | -1 (1.32873) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74597 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (1.70300) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93409 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (1.51489) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99978 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (1.44920) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14574 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (1.30323) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76540 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (1.68357) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65981 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (0.78916) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09228 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.64330) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81630 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.36733) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30039 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.85142) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74011 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.29113) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37166 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.07731) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37171 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.92274) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81241 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.36344) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49686 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.04788) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25590 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.80693) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.67340) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12550 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.67653) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47028 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.02131) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35552 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.90655) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51980 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.07083) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31470 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.86573) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13960 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.69062) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25952 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.81055) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99701 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.54804) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28908 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.15989) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56536 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.11638) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29365 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (0.15532) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83423 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.38526) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66106 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.21209) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83026 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.38129) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95764 HOMO: -6.56067 LUMO: 1.66806 factor:1 | -1 (0.49133) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08619 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (0.36278) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31485 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.13412) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11980 HOMO: -6.87360 LUMO: 1.75786 factor:1 | -1 (0.32918) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81297 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (1.63600) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05017 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (1.39880) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90116 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (1.54781) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21953 HOMO: -7.09129 LUMO: 2.31569 factor:1 | -1 (0.22945) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36513 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (0.08384) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85317 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.40420) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37674 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.92777) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36627 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.91730) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08398 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.63500) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15870 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.70973) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10743 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.65846) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41782 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (0.03116) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14426 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.30471) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29794 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.84897) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87619 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.42722) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77876 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (1.67021) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84769 HOMO: -6.19331 LUMO: 1.46941 factor:1 | -1 (1.60128) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04160 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (1.40737) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12076 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (1.32821) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88391 HOMO: -7.46408 LUMO: 0.31565 factor:1 | -1 (1.56506) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80533 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.35636) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82126 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (0.62771) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60364 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.15467) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74945 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (0.69952) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55045 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.89852) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80515 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.64382) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82163 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.37266) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95158 HOMO: -6.67767 LUMO: -0.48436 factor:1 | -1 (0.49740) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74790 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.70107) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05743 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.39154) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85451 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.59446) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97284 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (1.47614) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97926 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (1.46971) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77906 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.66992) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80622 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (1.64275) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02818 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (1.42079) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07531 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (1.37366) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84742 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (1.60155) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39598 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.94701) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59433 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-1.14535) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.71566) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07688 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.62790) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29737 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.84840) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82128 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.37231) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48784 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-2.03887) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59914 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.15017) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40172 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.95274) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39936 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.95038) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57844 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.12946) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91665 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.46767) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19620 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.74722) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90275 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.45378) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11451 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.66554) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83313 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.38416) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76674 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.31777) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04716 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.59819) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32991 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.88094) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98965 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.54068) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91452 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.46555) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20480 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.75582) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82531 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.37633) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34956 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.90059) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09532 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.64635) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88592 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (1.56305) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (1.35295) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32856 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.12041) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43958 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.00939) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15416 HOMO: -7.08584 LUMO: 1.98915 factor:1 | -1 (0.29481) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97988 HOMO: -6.69400 LUMO: 2.09256 factor:1 | -1 (0.46910) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69989 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.25092) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85641 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.40744) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00801 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.44096) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89966 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.54932) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61938 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.82959) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84072 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.60826) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18703 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.73805) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85184 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.40286) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79309 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.34412) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70988 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.26090) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02520 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.57623) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86433 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.41535) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30485 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.85588) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32193 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.87296) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71308 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.26410) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86132 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.41235) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15908 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.71011) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88705 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.43808) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69844 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.24947) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94068 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.49171) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92539 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.47642) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97012 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.52114) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24278 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.79381) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97368 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.52471) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72792 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.27894) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97192 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.52295) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81101 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.36204) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97627 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.52730) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-0.29900) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60985 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-0.16087) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53406 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-0.08509) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07345 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.62447) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22994 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.78097) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98874 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.53977) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14565 HOMO: -6.54434 LUMO: 2.32113 factor:1 | -1 (0.30333) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98023 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.46874) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01872 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-1.56974) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25799 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.80902) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90853 HOMO: -6.64502 LUMO: 2.13881 factor:1 | -1 (0.54045) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97588 HOMO: -6.95795 LUMO: 1.82316 factor:1 | -1 (0.47310) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85986 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.41089) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98838 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.53941) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51666 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-2.06768) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50969 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-2.06072) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17258 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.72361) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16273 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.71375) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16428 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.71531) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23139 HOMO: -6.63958 LUMO: 2.11977 factor:1 | -1 (0.21758) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36679 HOMO: -6.92802 LUMO: 1.82044 factor:1 | -1 (0.08218) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22146 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.22751) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39406 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (0.05491) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41776 HOMO: -6.93074 LUMO: 2.05446 factor:1 | -1 (0.03121) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57662 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.12765) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25767 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.80870) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.44746 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-1.99849) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03406 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-1.58509) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16117 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.71219) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14041 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-0.69144) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79733 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.34836) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98618 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.53721) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96272 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.51375) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76585 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.31688) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97045 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.52148) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01600 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-0.56703) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80667 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.35769) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99938 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.55040) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04783 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-1.59886) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82914 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.38017) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84985 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.40088) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82781 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.37884) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85630 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.40733) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54563 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.09665) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66261 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.21364) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74539 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.29641) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44394 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (0.00503) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94528 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.49631) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04194 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.40703) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01250 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (0.43647) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12399 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.32499) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.17334 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (2.27563) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98324 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.53427) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03013 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.58115) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.75234) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58005 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.13108) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26208 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.81310) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50399 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.05502) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08224 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-0.63326) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00407 HOMO: -6.98516 LUMO: 1.84765 factor:1 | -1 (0.44491) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71992 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.27094) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29503 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-0.84606) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16967 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.27930) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23955 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.20942) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99598 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (0.45299) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18159 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (0.26738) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87590 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (0.57307) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55056 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.89841) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38981 HOMO: -6.88448 LUMO: 2.54154 factor:1 | -1 (0.05916) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07960 HOMO: -6.87087 LUMO: 2.16058 factor:1 | -1 (0.36937) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81103 HOMO: -7.11306 LUMO: 2.04085 factor:1 | -1 (0.63794) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86881 HOMO: -6.66951 LUMO: 1.68438 factor:1 | -1 (1.58017) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87071 HOMO: -7.08312 LUMO: 2.19324 factor:1 | -1 (1.57826) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22817 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.77920) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89301 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.44404) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83970 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.39073) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03889 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.58992) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10194 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.65296) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11206 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.66309) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45403 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.00506) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12479 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.67582) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46160 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.01263) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27468 HOMO: -6.88720 LUMO: -0.67484 factor:1 | -1 (0.17429) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03679 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.58782) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37207 HOMO: -6.80285 LUMO: -0.57144 factor:1 | -1 (0.07690) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15014 HOMO: -6.76475 LUMO: -0.53062 factor:1 | -1 (0.29884) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05894 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.60997) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24344 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.79446) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57880 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.12983) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35806 HOMO: -6.64230 LUMO: 2.11977 factor:1 | -1 (0.09091) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21478 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.76581) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88566 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.43669) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78158 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.33260) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96996 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.52099) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21631 HOMO: -6.96067 LUMO: 2.20140 factor:1 | -1 (0.23266) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40078 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (0.04819) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03566 HOMO: -6.72665 LUMO: 2.46535 factor:1 | -1 (0.41331) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48575 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-1.03678) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97004 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.52107) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82587 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-1.37690) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32110 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.87212) | -1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89157 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.44259) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78269 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.33372) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78087 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.33190) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82299 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.37402) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69216 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.24319) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46718 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-0.01820) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89323 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.44425) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52603 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.07706) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36228 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.08670) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58160 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.13263) | 1 | 1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59118 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.14221) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79992 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.35095) | 1 | -1 |
| G: -5717.08328 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87731 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-0.42833) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.87518 HOMO: -6.72938 LUMO: 1.57282 factor:1 | -1 (2.35512) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.88217 HOMO: -6.17426 LUMO: 1.81228 factor:1 | -1 (2.34812) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.07427 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (1.15602) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87217 HOMO: -6.18515 LUMO: 2.01364 factor:1 | -1 (0.35813) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84066 HOMO: -7.05591 LUMO: 2.13337 factor:1 | -1 (0.38964) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.85009 HOMO: -6.90897 LUMO: 2.29664 factor:1 | -1 (2.38021) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31411 HOMO: -7.11034 LUMO: 2.17147 factor:1 | -1 (0.91618) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84819 HOMO: -6.82734 LUMO: 2.26671 factor:1 | -1 (0.38210) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80150 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (0.42880) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52938 HOMO: -6.62053 LUMO: 2.22861 factor:1 | -1 (0.70091) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.65359 HOMO: -6.80557 LUMO: 2.07079 factor:1 | -1 (1.57671) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54319 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (1.68711) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.51995 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (1.71034) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.32395 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (1.90635) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59485 HOMO: -6.51168 LUMO: 2.06534 factor:1 | -1 (0.63544) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.74863 HOMO: -6.50080 LUMO: 2.01636 factor:1 | -1 (1.48166) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74751 HOMO: -6.54434 LUMO: 1.84493 factor:1 | -1 (0.48278) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90411 HOMO: -6.47087 LUMO: 1.76330 factor:1 | -1 (0.32618) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.10181 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (1.12848) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.26620 HOMO: -6.59876 LUMO: 1.84493 factor:1 | -1 (1.96409) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.16764 HOMO: -6.41644 LUMO: 2.05174 factor:1 | -1 (2.06265) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77200 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (0.45829) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83295 HOMO: -6.90897 LUMO: 2.34018 factor:1 | -1 (0.39734) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.38723 HOMO: -6.97428 LUMO: 1.86126 factor:1 | -1 (0.84306) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.35103 HOMO: -7.13483 LUMO: 2.14698 factor:1 | -1 (2.87926) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.21513 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (2.01517) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.41683 HOMO: -6.87087 LUMO: 2.38916 factor:1 | -1 (2.81347) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65989 HOMO: -6.93074 LUMO: 2.42181 factor:1 | -1 (0.57041) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.99869 HOMO: -6.90081 LUMO: 2.00276 factor:1 | -1 (2.23161) | 1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50955 HOMO: -6.99333 LUMO: 2.03541 factor:1 | -1 (0.72075) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.55601 HOMO: -6.89264 LUMO: 1.57554 factor:1 | -1 (1.67429) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.08329 HOMO: -6.48175 LUMO: 1.85854 factor:1 | -1 (2.14701) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.07118 HOMO: -6.69400 LUMO: 1.62452 factor:1 | -1 (2.15911) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.70677 HOMO: -6.50896 LUMO: 1.88303 factor:1 | -1 (2.52353) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.60643 HOMO: -6.60420 LUMO: 2.05990 factor:1 | -1 (1.62387) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.75052 HOMO: -7.14299 LUMO: 2.07351 factor:1 | -1 (2.47977) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.84417 HOMO: -7.06408 LUMO: 1.81228 factor:1 | -1 (4.38612) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77580 HOMO: -6.67495 LUMO: 1.79595 factor:1 | -1 (2.45449) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.30284 HOMO: -6.45182 LUMO: 2.15786 factor:1 | -1 (2.92746) | -1 | -1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.56772 HOMO: -6.93346 LUMO: 2.45719 factor:1 | -1 (2.66258) | 1 | 1 |
| G: -6154.86460 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.45343 HOMO: -6.50080 LUMO: 2.08167 factor:1 | -1 (2.77687) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.78776 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (4.44253) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.69659 HOMO: -7.04231 LUMO: 0.54151 factor:1 | -1 (2.53371) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77841 HOMO: -6.79740 LUMO: 1.91296 factor:1 | -1 (2.45188) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.72726 HOMO: -7.35796 LUMO: -1.04220 factor:1 | -1 (2.50304) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.96322 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (4.26707) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.10646 HOMO: -6.45182 LUMO: -0.20409 factor:1 | -1 (3.12384) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.49272 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (2.73757) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.59144 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (2.63885) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.36297 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (4.86733) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21822 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (1.01207) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35857 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.12827) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42163 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (0.80867) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.10490) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48576 HOMO: -6.57155 LUMO: -0.53606 factor:1 | -1 (0.74453) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23750 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.00720) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63931 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.40901) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.66741 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.43711) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91248 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.68218) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76267 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.46763) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83619 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (0.39410) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16359 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.93330) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44961 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.21931) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83490 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.60461) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32219 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.09189) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97054 HOMO: -7.22462 LUMO: 0.52518 factor:1 | -1 (0.25976) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65096 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.42066) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40088 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.17059) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04528 HOMO: -6.71033 LUMO: 1.59187 factor:1 | -1 (0.18501) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87690 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.35339) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36951 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.13921) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73975 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.50945) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43677 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.20648) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16125 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.93096) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20208 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.02822) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.34191 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (1.88839) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32809 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.09780) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89828 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.66799) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40110 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.17081) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31650 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.08621) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32894 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.09864) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59589 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.63441) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30815 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.07785) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09236 HOMO: -6.35114 LUMO: 1.92112 factor:1 | -1 (0.13793) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44302 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.78728) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31627 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.08598) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31630 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.08601) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10022 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.86992) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54515 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.31485) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93077 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.70048) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86347 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.63317) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29546 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.06516) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.87560 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.64531) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47921 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.75109) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17737 HOMO: -7.20285 LUMO: 0.53879 factor:1 | -1 (0.05293) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98327 HOMO: -6.46815 LUMO: -0.21769 factor:1 | -1 (0.24702) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -6.57971 LUMO: -0.18776 factor:1 | -1 (0.67686) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73384 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.50355) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74705 HOMO: -6.67495 LUMO: 2.04358 factor:1 | -1 (0.48325) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54025 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.30996) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84982 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.61952) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.58107 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.35077) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71248 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.48219) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17235 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.94206) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.40556 LUMO: 1.45581 factor:1 | -1 (1.50822) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95228 HOMO: -6.94979 LUMO: 2.16603 factor:1 | -1 (0.27802) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01535 HOMO: -6.84911 LUMO: 1.89935 factor:1 | -1 (0.21494) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94387 HOMO: -6.22052 LUMO: 1.57282 factor:1 | -1 (0.28643) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.05453 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.82423) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84503 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.61473) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69392 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.46363) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07129 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.84100) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40061 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.17032) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.62921 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.39892) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.18253 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.95224) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45726 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.22696) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.82671 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.59641) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34076 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.11047) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77969 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.54940) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06797 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.83768) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07151 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.84121) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14958 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.91928) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.56572 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.33543) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46958 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.23929) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99972 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.76943) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29238 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.06209) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18776 HOMO: -6.50080 LUMO: 1.87759 factor:1 | -1 (0.04253) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79586 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.56556) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69151 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.53879) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74770 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.48259) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86564 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.63535) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38257 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.15227) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40821 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.82208) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.13865 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.09165) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03720 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (0.19309) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23460 HOMO: -6.66407 LUMO: 2.07623 factor:1 | -1 (0.99569) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.39191 HOMO: -6.52529 LUMO: 1.70071 factor:1 | -1 (0.83838) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83671 HOMO: -6.58788 LUMO: 1.57282 factor:1 | -1 (0.39359) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15497 HOMO: -6.55250 LUMO: 1.95378 factor:1 | -1 (0.07532) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80302 HOMO: -6.24773 LUMO: 1.77962 factor:1 | -1 (0.42727) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.15910 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.92881) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49144 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.26115) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.27682 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.04652) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78677 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.55647) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25154 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.02124) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.04709 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.81680) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07515 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.84486) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60791 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.37761) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55827 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.32798) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54790 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.31760) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25363 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.02334) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10533 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.87504) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.13344 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.90315) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78127 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.55098) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91485 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.68456) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05337 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.17693) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58105 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.35075) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18431 HOMO: -6.60420 LUMO: -0.22585 factor:1 | -1 (0.04599) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44478 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.21448) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07043 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.15987) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85608 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.37421) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06997 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (0.16033) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79886 HOMO: -6.53890 LUMO: -0.46531 factor:1 | -1 (0.43144) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53733 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.69297) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60179 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.62850) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77829 HOMO: -6.75659 LUMO: -0.45715 factor:1 | -1 (0.45201) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98814 HOMO: -6.66135 LUMO: -0.41906 factor:1 | -1 (0.24215) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30297 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.07267) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99387 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.76358) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64995 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.41965) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39494 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.16465) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39361 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.16331) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.95427 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.72398) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29886 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.06856) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30302 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.07273) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97895 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.74866) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63451 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.40422) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30942 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.07912) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.61288 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.38258) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01107 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.78078) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28224 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.05195) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27786 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.04757) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96795 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (0.26234) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83304 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.39726) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98569 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (0.24460) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82947 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.40082) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.78305 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (0.44725) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79540 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (0.43489) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67292 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.55737) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63710 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.40680) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84701 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.61672) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10375 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.87346) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25720 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.02690) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39218 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.16188) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14016 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.90987) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69169 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.46140) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44305 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.21276) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99513 HOMO: -6.88992 LUMO: 1.65173 factor:1 | -1 (0.23516) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.04942) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51562 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.28533) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71351 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.48322) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.57449 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.34420) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94361 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.71332) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44835 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (0.78195) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.46999 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (1.76030) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.36678 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.13648) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54997 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.31968) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47264 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.24234) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55436 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (0.67593) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04998 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.81969) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16052 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.06977) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12726 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.89697) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.11978 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (2.11052) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12572 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.10457) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.41513 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (1.81516) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28872 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.05842) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22945 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.00084) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98977 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.24052) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24398 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.01369) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82879 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (0.40150) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.88681 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (0.34349) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79616 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (0.43413) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76634 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.46395) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35993 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.12964) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07467 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (0.15562) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18072 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (0.04958) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72514 HOMO: -6.56611 LUMO: -0.77008 factor:1 | -1 (0.50515) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44061 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.21032) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59989 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (0.63041) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35830 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.12800) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09492 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (0.13538) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28183 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.05154) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36037 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.13007) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95590 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (0.27440) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25574 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.02544) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66800 HOMO: -6.65046 LUMO: -0.41361 factor:1 | -1 (0.56230) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89349 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.66320) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.19107 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.96078) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33356 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.10327) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96479 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.26550) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92348 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.69318) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03424 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (0.19606) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98711 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (0.24319) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05652 HOMO: -6.67495 LUMO: -0.27211 factor:1 | -1 (0.17377) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25555 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.02525) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35601 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.12572) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42031 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.19002) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91919 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (0.31111) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75128 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.52099) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49695 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (0.73335) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26763 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.03733) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09364 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (0.13666) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35743 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.12713) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42420 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.19391) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34847 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.11817) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59556 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.63473) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04903 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.81874) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77520 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.54491) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25053 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.02024) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50720 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.27690) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16367 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.93338) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10555 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.87525) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38967 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.15938) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82103 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.59073) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46937 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.23908) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.80780 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.57751) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (0.04942) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97074 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.74045) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82144 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.59114) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04654 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.18376) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64853 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.41824) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (1.50822) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43487 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.20458) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36078 HOMO: -6.80557 LUMO: 2.23678 factor:1 | -1 (0.86951) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80487 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.42542) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34793 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.11763) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.42662 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.19632) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25010 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.01981) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.99819 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.76790) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58861 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.35832) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54445 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.31416) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79126 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.56096) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37785 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.14756) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.85732 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.62702) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89041 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.66011) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77335 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.54306) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.03654 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.80625) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76640 HOMO: -7.07224 LUMO: 2.13337 factor:1 | -1 (0.46390) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (0.67686) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49893 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.26863) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92511 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.69482) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.55369 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.32340) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71025 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.47995) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83292 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.60262) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95641 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (0.27388) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32532 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.09502) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75290 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.47740) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (0.36627) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08675 HOMO: -7.46408 LUMO: 0.31565 factor:1 | -1 (0.14354) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91029 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.32001) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73869 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (0.49160) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89257 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.66227) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.32784 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.09754) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81137 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.58107) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33867 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.10837) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93684 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.70654) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85096 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.62066) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33086 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.10056) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.71783 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.48754) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85942 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.62913) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76026 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.52996) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75708 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.52679) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21995 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.98965) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23091 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-1.00062) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12071 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.89041) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06610 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.16419) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02177 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.20852) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25293 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.02263) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62795 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-1.39766) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.92230 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.69200) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25056 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.02026) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.81732 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.58702) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.77250 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.54221) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99099 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.76069) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49271 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.26242) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07720 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (0.15309) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09756 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (0.13274) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00743 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (0.22286) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61344 HOMO: -6.54706 LUMO: 1.91024 factor:1 | -1 (0.61685) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64305 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.58725) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45182 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.22153) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45045 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.22016) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60037 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.37007) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45634 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.22604) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02215 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.79185) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93355 HOMO: -7.10761 LUMO: 2.20956 factor:1 | -1 (0.29674) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28956 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.05927) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62529 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.39499) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91661 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-1.68632) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.01582 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.78553) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08696 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.85667) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66909 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.56121) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64291 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.58738) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61140 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.61890) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58473 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.64556) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74925 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.48104) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69509 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.46480) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56617 HOMO: -6.69400 LUMO: 2.09256 factor:1 | -1 (0.66412) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15503 HOMO: -6.62869 LUMO: 2.16331 factor:1 | -1 (0.07527) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30668 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.07638) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31471 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.91558) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14679 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (1.08350) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.99327 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (1.23703) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40322 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.17293) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25295 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.02266) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12569 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.89539) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98010 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.74981) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54766 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.31737) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34483 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.11453) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.52034 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.29005) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.74116 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.51087) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.53315 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.30285) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11791 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (0.11238) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53259 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.30229) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72383 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.49353) | 1 | 1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02079 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.79049) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53457 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.30428) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72415 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.49386) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.88576 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.65547) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.22351 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.99322) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95425 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.72396) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31158 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.08128) | -1 | -1 |
| G: -6154.86460 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46703 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.23674) | -1 | -1 |