乙二醇作为反应物的反应表19-18

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: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13961 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.96489) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27841 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.10369) | 1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97460 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.79988) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27856 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.10384) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21545 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.04074) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16720 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.99248) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01857 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.84385) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.26833 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.09361) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79623 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.62151) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12683 HOMO: -6.69400 LUMO: 1.67622 factor:1 | -1 (0.04789) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93748 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.76276) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23750 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.06278) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58169 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.40697) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47402 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.29930) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68390 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.50918) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25066 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.07594) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21387 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.03915) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32672 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.15200) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12079 HOMO: -6.58788 LUMO: 1.73881 factor:1 | -1 (0.05393) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14751 HOMO: -6.64502 LUMO: 1.70343 factor:1 | -1 (0.02721) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01121 HOMO: -6.73754 LUMO: 1.60819 factor:1 | -1 (0.16351) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16767 HOMO: -6.80829 LUMO: 2.45991 factor:1 | -1 (0.00705) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49067 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.31595) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59739 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.42267) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32950 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.15478) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45551 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.28079) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89106 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.71634) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53094 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.35622) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50436 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.32964) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27301 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.09829) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21431 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.03959) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38368 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.20896) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49614 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.32142) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63780 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.46308) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30634 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.13162) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48624 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.31152) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76942 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.59470) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03038 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.85566) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93582 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.76110) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08429 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.90957) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.22957 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-1.05485) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07806 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.90334) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10723 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.93251) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18862 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-1.01390) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23116 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.05644) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23325 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.05853) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28166 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.10694) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18383 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.00911) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.26250 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.08778) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22718 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.05246) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29886 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.12414) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85261 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.67789) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02157 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.84685) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99482 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.82010) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19754 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-1.02282) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37815 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.20343) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55296 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.37824) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60594 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.43122) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.96124 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.78652) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95985 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.78513) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54487 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-1.37015) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53323 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.35851) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28160 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.10688) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30637 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.13165) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20590 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-1.03118) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02222 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.84750) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92622 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.75150) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61620 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.44148) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50180 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.32708) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67187 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.49715) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58308 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.40836) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70667 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.53196) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37992 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.20520) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.77664 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.60192) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67761 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.50289) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58455 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.40983) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79021 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.61549) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90905 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.73433) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79786 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.62314) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75010 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.57538) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.78638 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-0.61166) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53296 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.35824) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50983 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.33511) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.73296 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-0.55824) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49821 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.32349) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42817 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-0.25345) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60591 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-0.43119) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48539 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-0.31067) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66458 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.48986) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50885 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.33413) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68012 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.50540) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40577 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.23105) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44323 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.26851) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14924 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.97452) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20268 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.02796) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29578 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.12106) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29026 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.11554) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13349 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (0.04123) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20144 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-0.02672) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25815 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-0.08343) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29943 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.12471) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.08242 HOMO: -6.86543 LUMO: -0.93063 factor:1 | -1 (0.09230) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32471 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.14999) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59358 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.41886) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34732 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.17260) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36525 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.19053) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28512 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.11040) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37837 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-0.20365) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09744 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.07728) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13080 HOMO: -7.07768 LUMO: 0.45987 factor:1 | -1 (0.04392) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00590 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.16882) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57914 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.40442) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61224 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.43752) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44655 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-1.27183) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13210 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.95738) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32146 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.14674) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54960 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-1.37488) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54642 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.37170) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66071 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.48600) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97122 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.79650) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40087 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.22615) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48583 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.31111) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36656 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.19184) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66852 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.49381) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56618 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.39146) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74055 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.56583) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46202 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.28730) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75838 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.58366) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.72142 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.54670) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99577 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.82105) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60534 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.43062) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.78534 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.61062) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84281 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.66809) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49037 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.31565) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69663 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.52191) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95555 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.78083) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06110 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.88638) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98818 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.81346) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81307 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.63835) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.15210 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.97738) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53864 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.36393) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43649 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.26177) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84045 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.66573) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79778 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.62306) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06249 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.88777) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84504 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.67033) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82085 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.64613) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93068 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.75596) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86788 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.69316) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.94279 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.76807) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81326 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.63854) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63895 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.46423) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86567 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.69095) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47121 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.29650) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61266 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.43794) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79598 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.62126) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92970 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.75498) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40074 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.22602) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07615 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-0.90143) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86281 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-0.68809) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.39444 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-1.21972) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34523 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.17051) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28113 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-1.10641) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49225 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.31753) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.39515 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-1.22043) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33766 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.16294) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28876 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.11404) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26007 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-1.08535) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.26501 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.09029) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60120 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.42648) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54977 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.37505) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53005 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.35533) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87481 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.70009) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10891 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.93419) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90192 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.72720) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19561 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.02089) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85443 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.67971) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64031 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.46559) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92257 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.74785) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.45523 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.28051) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12832 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.95360) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.77947 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.60475) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88518 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.71046) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59258 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-0.41786) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.42043 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.24571) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38362 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-0.20890) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31298 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-0.13826) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40248 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.22776) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64583 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.47111) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49908 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.32436) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76311 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.58839) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42008 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.24537) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64409 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-0.46937) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54736 HOMO: -6.58243 LUMO: 2.11705 factor:1 | -1 (0.62736) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27399 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.09927) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.08797 HOMO: -6.50624 LUMO: 2.55787 factor:1 | -1 (0.08675) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14354 HOMO: -6.45454 LUMO: 1.87214 factor:1 | -1 (0.03118) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99539 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.82067) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43942 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.26470) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.43917 HOMO: -6.75114 LUMO: 1.84493 factor:1 | -1 (0.73555) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44344 HOMO: -6.06270 LUMO: 1.65717 factor:1 | -1 (0.73128) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68266 HOMO: -5.89671 LUMO: 1.71704 factor:1 | -1 (0.49206) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50330 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-0.32858) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63478 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.46006) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58526 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.41054) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53264 HOMO: -6.05725 LUMO: 2.03541 factor:1 | -1 (0.64208) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39958 HOMO: -6.80829 LUMO: 1.90480 factor:1 | -1 (0.77514) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42441 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.24969) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68202 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.50730) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.85482 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (0.31990) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67029 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-0.49557) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.13334 HOMO: -7.20830 LUMO: 0.49797 factor:1 | -1 (1.04138) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18441 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-0.00969) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43987 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.26515) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21175 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.03703) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68346 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.50874) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52629 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.35157) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.00143 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.82671) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27483 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.10011) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06154 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.88682) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14087 HOMO: -6.48175 LUMO: 1.91296 factor:1 | -1 (0.03385) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.85780 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.68308) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.62933 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-1.45461) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87607 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.70135) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49245 HOMO: -6.06542 LUMO: 1.92112 factor:1 | -1 (0.68227) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40371 HOMO: -6.90353 LUMO: 1.83133 factor:1 | -1 (0.77101) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.34273 HOMO: -6.37019 LUMO: 1.92929 factor:1 | -1 (0.83199) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.92900 HOMO: -6.61509 LUMO: 2.11160 factor:1 | -1 (0.24572) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.67316 HOMO: -6.82734 LUMO: 1.77146 factor:1 | -1 (0.50156) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56983 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-0.39511) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30770 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.13298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07743 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.90271) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.47093 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.29621) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.40465 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.22993) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85917 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.68445) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95264 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.77792) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.78017 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.60545) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95952 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.78480) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.38013 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-1.20541) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.89832 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-1.72360) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.30309 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-2.12837) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49027 HOMO: -6.03276 LUMO: 1.67078 factor:1 | -1 (0.68445) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.05802 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (1.11670) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21916 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.95556) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75977 HOMO: -6.07086 LUMO: 2.01908 factor:1 | -1 (0.41495) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51726 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.34254) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45230 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.27758) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58798 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.41326) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89949 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.72478) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98238 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.80766) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99030 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.81558) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11711 HOMO: -7.04231 LUMO: 0.64219 factor:1 | -1 (0.05761) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76493 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.59021) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16721 HOMO: -6.83822 LUMO: -0.97417 factor:1 | -1 (0.00751) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07978 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (0.09494) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82684 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.65212) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68631 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.51159) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53256 HOMO: -6.96611 LUMO: 1.24900 factor:1 | -1 (0.64216) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56105 HOMO: -7.21102 LUMO: 0.82995 factor:1 | -1 (0.61367) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15929 HOMO: -6.88448 LUMO: 0.81634 factor:1 | -1 (0.01543) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.78780 HOMO: -7.04231 LUMO: 1.10750 factor:1 | -1 (0.38692) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98702 HOMO: -6.83550 LUMO: -0.98777 factor:1 | -1 (0.18770) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06843 HOMO: -6.82189 LUMO: 0.93879 factor:1 | -1 (0.10629) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13047 HOMO: -6.81101 LUMO: 0.70750 factor:1 | -1 (0.04425) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99912 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.82440) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.56655 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.39184) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95155 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-0.77683) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18147 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.00675) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27293 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.09821) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.69701 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-1.52229) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.00799 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.83327) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.80487 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-1.63015) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46553 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.29081) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88962 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.71490) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.19935 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.02463) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53850 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-1.36378) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98124 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.80652) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03952 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.86481) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.88362 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.70890) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13651 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.96179) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12305 HOMO: -7.24095 LUMO: 0.37280 factor:1 | -1 (0.05167) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15668 HOMO: -6.81101 LUMO: -0.74831 factor:1 | -1 (0.01804) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50194 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.32722) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33119 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.15647) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.17143 HOMO: -6.66679 LUMO: -0.47076 factor:1 | -1 (0.00329) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80175 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.62703) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08306 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.90834) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86973 HOMO: -6.53617 LUMO: -0.35375 factor:1 | -1 (0.30499) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31619 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.14147) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66108 HOMO: -6.69400 LUMO: -0.67484 factor:1 | -1 (0.51364) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28419 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-0.10947) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43655 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.26183) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56866 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.39394) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07806 HOMO: -6.80557 LUMO: -0.56600 factor:1 | -1 (0.09665) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84013 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.33459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76355 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.58883) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51527 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.34055) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43595 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.26123) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07604 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-0.90132) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11764 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (1.05708) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03132 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (0.14340) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.16904 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (1.00568) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.17466 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.99994) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.91770 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.74298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75008 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.57536) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03834 HOMO: -7.23279 LUMO: 0.46804 factor:1 | -1 (0.13638) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90945 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.73473) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96228 HOMO: -6.83278 LUMO: -0.59321 factor:1 | -1 (0.21244) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.92950 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (1.24522) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90053 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.72581) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29365 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.11893) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74757 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.57285) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16070 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.98598) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41608 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.24136) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.69135 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-1.51663) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.02833 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.85361) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20714 HOMO: -7.00965 LUMO: -1.05036 factor:1 | -1 (0.96758) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09461 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.08011) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11133 HOMO: -6.91713 LUMO: 0.93607 factor:1 | -1 (1.06339) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35143 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.17671) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12857 HOMO: -6.98516 LUMO: 1.52384 factor:1 | -1 (0.04615) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97318 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.79846) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35104 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.17632) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67704 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.50232) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09830 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.92358) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38544 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.21072) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.10922 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (0.06550) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50922 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-1.33450) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.06743 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-1.89272) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10266 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.92794) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65165 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.47693) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99798 HOMO: -7.37701 LUMO: 0.14150 factor:1 | -1 (0.17674) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98957 HOMO: -6.74842 LUMO: -0.68028 factor:1 | -1 (0.18515) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.52872 HOMO: -6.65046 LUMO: -0.52518 factor:1 | -1 (0.64600) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.41830 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (0.75642) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61218 HOMO: -7.00965 LUMO: -1.00682 factor:1 | -1 (0.56254) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33818 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.16346) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37995 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.20523) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50618 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.33146) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62142 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-0.44670) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18557 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.01085) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.41654 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.24182) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93792 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.76320) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35209 HOMO: -6.97700 LUMO: -0.98505 factor:1 | -1 (0.82263) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30599 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.13127) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22218 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-0.04746) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69794 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-0.52322) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53244 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.35772) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29428 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.11956) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.77370 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.59898) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.82432 HOMO: -6.70761 LUMO: -0.63403 factor:1 | -1 (0.35040) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45366 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.27894) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34331 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.16859) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58423 HOMO: -6.98516 LUMO: 0.38096 factor:1 | -1 (0.59049) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23038 HOMO: -6.47087 LUMO: -0.40001 factor:1 | -1 (0.94434) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42278 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-0.24806) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13964 HOMO: -6.89809 LUMO: 0.14966 factor:1 | -1 (0.03508) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.17192 HOMO: -6.76203 LUMO: 2.11432 factor:1 | -1 (0.00280) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.11517 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.94045) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68439 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.50967) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57991 HOMO: -6.83550 LUMO: 1.74425 factor:1 | -1 (0.59481) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35750 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.18278) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68442 HOMO: -6.68584 LUMO: 2.11160 factor:1 | -1 (0.49029) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.51789 HOMO: -6.36202 LUMO: 1.85037 factor:1 | -1 (0.65683) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25431 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.07959) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34130 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.16658) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43628 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.26156) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16272 HOMO: -6.63686 LUMO: 2.22317 factor:1 | -1 (0.01200) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09754 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.92282) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79163 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.61691) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49848 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.32376) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75779 HOMO: -6.56067 LUMO: 2.27487 factor:1 | -1 (0.41693) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68161 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.50689) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51698 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.34226) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52131 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.34659) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98489 HOMO: -6.23413 LUMO: 1.80956 factor:1 | -1 (0.18983) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15535 HOMO: -6.74298 LUMO: 2.16875 factor:1 | -1 (0.01937) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.89145 HOMO: -6.81645 LUMO: 2.50073 factor:1 | -1 (0.28327) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00372 HOMO: -6.71033 LUMO: 1.96466 factor:1 | -1 (0.17100) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44805 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-1.27333) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70485 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.53013) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94457 HOMO: -6.73210 LUMO: 2.26127 factor:1 | -1 (0.23015) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64194 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.46722) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52787 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.35315) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60605 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.43133) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33856 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.16384) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.56933 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.39461) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81789 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.64317) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95302 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.77830) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98948 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.81476) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53322 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.35850) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53575 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.36103) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02848 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.85376) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.60664 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-1.43192) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.69774 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-1.52302) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30833 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.13361) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18316 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.00844) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33014 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-1.15542) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03797 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.86325) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18247 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-1.00775) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.69766 HOMO: -6.13345 LUMO: 0.67756 factor:1 | -1 (1.47706) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.69426 HOMO: -6.48719 LUMO: 0.52790 factor:1 | -1 (1.48046) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.86822 HOMO: -6.35930 LUMO: 0.74015 factor:1 | -1 (1.30650) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.26432 HOMO: -6.41644 LUMO: 0.22313 factor:1 | -1 (1.91040) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05795 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.88323) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24097 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.06625) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75744 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.58272) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58673 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.41201) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.94902 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-0.77430) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67614 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.50142) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.33840 HOMO: -6.46270 LUMO: -0.46259 factor:1 | -1 (0.83631) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45634 HOMO: -6.36202 LUMO: -0.29660 factor:1 | -1 (0.71838) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58989 HOMO: -6.28583 LUMO: 0.40545 factor:1 | -1 (0.58483) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.38894 HOMO: -6.70761 LUMO: 0.41906 factor:1 | -1 (0.78578) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53104 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-1.35632) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54838 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-1.37366) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21513 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.04041) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50332 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.32860) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.76038 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.58566) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10720 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.93248) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93936 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.76464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53115 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-1.35643) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54171 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.36699) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99770 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.82298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19311 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-1.01839) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.81094 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.63622) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.48956 HOMO: -6.73482 LUMO: 2.20956 factor:1 | -1 (0.68516) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49057 HOMO: -6.74026 LUMO: 1.76602 factor:1 | -1 (0.68415) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34609 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.17137) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53377 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.35905) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56186 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.38714) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67941 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.50469) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61269 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-0.43797) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.46662 HOMO: -6.53073 LUMO: 2.08983 factor:1 | -1 (0.70809) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.52842 HOMO: -6.69944 LUMO: 2.20684 factor:1 | -1 (0.64630) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43010 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.25538) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86048 HOMO: -6.78380 LUMO: 1.95922 factor:1 | -1 (0.31424) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54823 HOMO: -6.93618 LUMO: 1.76058 factor:1 | -1 (0.62649) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57895 HOMO: -6.93346 LUMO: 1.79595 factor:1 | -1 (0.59577) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23220 HOMO: -6.29671 LUMO: 1.75241 factor:1 | -1 (0.94252) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35066 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-1.17594) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54722 HOMO: -6.87360 LUMO: 1.91024 factor:1 | -1 (0.62749) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44304 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-1.26832) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.60718 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (1.56754) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.51178 HOMO: -6.72665 LUMO: 2.12521 factor:1 | -1 (1.66294) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.08134 HOMO: -6.67767 LUMO: 2.43814 factor:1 | -1 (1.09338) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34574 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.17102) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53611 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.36139) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20238 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.02767) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84605 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.67133) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03991 HOMO: -6.78924 LUMO: 2.01364 factor:1 | -1 (0.13481) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.73413 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.55941) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62929 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.45457) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.34600 HOMO: -6.05998 LUMO: 2.12521 factor:1 | -1 (0.82872) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56339 HOMO: -6.67223 LUMO: 1.91840 factor:1 | -1 (0.61133) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07559 HOMO: -6.79196 LUMO: 2.18507 factor:1 | -1 (0.09913) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56964 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-0.39492) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89277 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.71805) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67984 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-0.50512) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09357 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.91885) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12598 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.95126) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.55640 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-1.38169) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22687 HOMO: -6.97700 LUMO: 1.91024 factor:1 | -1 (0.94785) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36785 HOMO: -6.20420 LUMO: 1.81772 factor:1 | -1 (0.80687) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55351 HOMO: -7.09129 LUMO: 2.10344 factor:1 | -1 (0.62121) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.45278 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-1.27806) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29203 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.11731) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20762 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.03290) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38719 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.21247) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55913 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.38442) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92899 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.75427) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.73675 HOMO: -6.30216 LUMO: 2.24222 factor:1 | -1 (0.43797) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87624 HOMO: -7.18108 LUMO: 2.10072 factor:1 | -1 (0.29848) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21821 HOMO: -6.54162 LUMO: 2.35378 factor:1 | -1 (0.95651) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24510 HOMO: -5.98650 LUMO: 1.48302 factor:1 | -1 (0.92962) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40856 HOMO: -7.15115 LUMO: 2.14970 factor:1 | -1 (0.76616) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69106 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.51634) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36608 HOMO: -7.06952 LUMO: 2.14970 factor:1 | -1 (0.80864) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.34581 HOMO: -6.93618 LUMO: 1.86942 factor:1 | -1 (0.82891) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.82576 HOMO: -6.63141 LUMO: 1.92657 factor:1 | -1 (0.34896) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40385 HOMO: -6.51441 LUMO: -0.44355 factor:1 | -1 (0.77087) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75260 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.57788) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75268 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.57796) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16630 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.99158) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.89987 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-1.72515) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08913 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.91441) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.46508 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.29036) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.71673 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.54201) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.34464 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.16992) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.34532 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.17060) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61466 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.43994) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.86006 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.68534) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.89168 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.71696) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16630 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.99158) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32018 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-1.14546) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09482 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.92010) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.80577 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.63105) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.89173 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.71701) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39881 HOMO: -6.24773 LUMO: -0.53879 factor:1 | -1 (0.77591) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55392 HOMO: -6.96067 LUMO: -0.67212 factor:1 | -1 (0.62080) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55367 HOMO: -7.24095 LUMO: -0.09252 factor:1 | -1 (0.62105) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.17240 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.99768) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88899 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.71427) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43494 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.26022) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25189 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.07717) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.24765 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.07293) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.87968 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-1.70496) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.38535 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.21063) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29077 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.11605) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61284 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-1.43812) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34272 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.16800) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65352 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.47880) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.49076 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-2.31604) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.63235 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.45763) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.50080 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-2.32608) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75796 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.58324) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49251 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.31779) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.51066 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.33594) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.27865 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-2.10393) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.93492 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.76020) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.45420 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.27948) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61287 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.43815) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.87663 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.70191) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35047 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.17575) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65317 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.47845) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40455 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-0.22983) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35606 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.18134) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52964 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.35492) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58534 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.41062) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.96502 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.79030) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06818 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.89346) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82020 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.64548) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04083 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.86611) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58661 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.41189) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85775 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.68303) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49140 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.31668) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67388 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.49916) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.79755 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.62283) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53453 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-1.35981) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75869 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.58397) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.55989 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-1.38517) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29482 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.12010) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61043 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.43571) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05724 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.88252) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.08289 HOMO: -6.56611 LUMO: 1.94561 factor:1 | -1 (1.09183) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.63577 HOMO: -6.67767 LUMO: 1.51840 factor:1 | -1 (0.53895) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49806 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.32334) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68726 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.51254) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14149 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.96677) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.77219 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.59747) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.95919 HOMO: -6.24773 LUMO: 1.98915 factor:1 | -1 (1.21553) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.63833 HOMO: -6.53617 LUMO: 2.42726 factor:1 | -1 (0.53639) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10385 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.92913) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75012 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.57540) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58499 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.41027) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32543 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.15072) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01430 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.83958) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87000 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.69528) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47554 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.30082) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22356 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.04884) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95087 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.77615) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.46320 HOMO: -6.70761 LUMO: 1.97555 factor:1 | -1 (0.71152) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96889 HOMO: -6.15794 LUMO: 2.00548 factor:1 | -1 (0.20583) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84383 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (0.33089) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84274 HOMO: -6.25590 LUMO: 1.86670 factor:1 | -1 (0.33198) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79898 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.62426) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43101 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.25630) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49420 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.31948) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67179 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.49707) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11115 HOMO: -6.81917 LUMO: 2.34834 factor:1 | -1 (0.06357) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.57224 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.39752) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.91868 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.74396) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.71801 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.54329) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04848 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.87376) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76972 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.59500) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.62871 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.45399) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35586 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.18114) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03746 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.86274) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63865 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.46393) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43918 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.26446) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49420 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.31948) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04933 HOMO: -6.77564 LUMO: -0.80001 factor:1 | -1 (0.12539) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05925 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.88453) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70929 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.53457) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88714 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-0.71242) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90344 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.72872) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24480 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.92992) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37776 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.20304) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07338 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.89866) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02516 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.85044) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04203 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.86731) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01942 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.84470) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.84313 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.66841) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16606 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.99134) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69362 HOMO: -6.15249 LUMO: 0.66396 factor:1 | -1 (0.48110) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43744 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.26272) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26437 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.08965) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69596 HOMO: -6.32393 LUMO: 0.47620 factor:1 | -1 (0.47876) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30012 HOMO: -6.32937 LUMO: 0.45987 factor:1 | -1 (0.87460) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21220 HOMO: -7.37429 LUMO: 0.09252 factor:1 | -1 (0.96252) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.17579 HOMO: -6.54434 LUMO: -0.39729 factor:1 | -1 (0.99893) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40200 HOMO: -7.35524 LUMO: 0.28028 factor:1 | -1 (0.77272) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.41726 HOMO: -6.95523 LUMO: -0.86804 factor:1 | -1 (0.75746) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.29857 HOMO: -6.63958 LUMO: -0.65307 factor:1 | -1 (0.87615) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.19870 HOMO: -6.73482 LUMO: -0.67212 factor:1 | -1 (0.97602) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31791 HOMO: -6.37835 LUMO: -0.53606 factor:1 | -1 (0.85680) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30703 HOMO: -6.71849 LUMO: -0.61226 factor:1 | -1 (0.86769) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.28616 HOMO: -6.68584 LUMO: -1.11022 factor:1 | -1 (0.88856) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.47345 HOMO: -6.80285 LUMO: -0.79185 factor:1 | -1 (0.70126) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.89539 HOMO: -7.14571 LUMO: -0.94696 factor:1 | -1 (0.27932) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09796 HOMO: -7.16204 LUMO: -0.66124 factor:1 | -1 (0.07676) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95841 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.78369) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.15253 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.97781) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80216 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.62744) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06505 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-0.89033) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16424 HOMO: -6.87360 LUMO: -0.77552 factor:1 | -1 (0.01048) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70782 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-0.53310) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.17156 HOMO: -6.65318 LUMO: -0.46259 factor:1 | -1 (0.00316) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93462 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.75991) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06916 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-0.89444) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31576 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.14104) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25458 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.07986) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34320 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.16848) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36982 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.19510) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33139 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-1.15667) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65462 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.47990) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10078 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.92606) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04669 HOMO: -6.52257 LUMO: -0.64491 factor:1 | -1 (0.12803) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53532 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.36060) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33012 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-1.15540) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30465 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.12993) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66829 HOMO: -6.43277 LUMO: 1.76330 factor:1 | -1 (0.50643) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75613 HOMO: -6.48175 LUMO: 1.77962 factor:1 | -1 (0.41859) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35483 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.18011) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04938 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.87466) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.30900 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.13428) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14657 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.97185) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02410 HOMO: -6.78108 LUMO: 2.16875 factor:1 | -1 (0.15062) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02868 HOMO: -6.34297 LUMO: 2.10344 factor:1 | -1 (0.14604) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69644 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.52172) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82826 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.65354) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.30375 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-1.12903) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16334 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.98862) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14750 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.97278) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93566 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.76094) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01928 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.84456) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32143 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.14672) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53913 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.36441) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02970 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.85498) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33589 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.16117) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74583 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.57111) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08644 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.91172) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99101 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.81629) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.95560 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.78088) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.40067 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.22595) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49929 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-1.32457) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62142 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.44670) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74575 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.57103) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93786 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.76314) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13945 HOMO: -6.72393 LUMO: 2.06534 factor:1 | -1 (0.03527) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.00673 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.83202) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12204 HOMO: -6.31304 LUMO: 1.87759 factor:1 | -1 (0.05268) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.73609 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.56137) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07199 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.89727) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.52933 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.35461) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.40691 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.23219) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33265 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.15793) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25507 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.08035) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19874 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.02402) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.85304 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.67832) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.00962 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.83490) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.30290 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.12818) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04394 HOMO: -6.61781 LUMO: 1.86126 factor:1 | -1 (0.13078) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79351 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.61879) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07006 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.89534) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15034 HOMO: -6.52529 LUMO: 2.05174 factor:1 | -1 (0.02438) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93812 HOMO: -6.80285 LUMO: 2.13609 factor:1 | -1 (0.23660) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76221 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.58749) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92480 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.75008) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04721 HOMO: -6.40828 LUMO: 1.99732 factor:1 | -1 (0.12751) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95605 HOMO: -5.97562 LUMO: 1.56465 factor:1 | -1 (0.21867) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86336 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.68864) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98176 HOMO: -6.68584 LUMO: 2.09528 factor:1 | -1 (0.19296) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.62334 HOMO: -6.86543 LUMO: 1.95106 factor:1 | -1 (1.55138) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45152 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (0.72320) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.82672 HOMO: -6.87632 LUMO: 2.08439 factor:1 | -1 (1.34800) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86497 HOMO: -6.33753 LUMO: 2.16603 factor:1 | -1 (0.30975) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.73293 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.55821) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.11610 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.94138) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.85477 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-2.68005) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.14491 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.97019) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.98781 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.81309) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.21568 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-2.04096) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50571 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.33099) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.28902 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-2.11430) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.72988 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.55516) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.77053 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-1.59581) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03664 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.86192) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52613 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.35141) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59462 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.41990) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03468 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.85996) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.42745 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-1.25273) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74806 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.57334) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96808 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (0.20664) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83617 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.66145) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.17467 HOMO: -6.95251 LUMO: 0.90614 factor:1 | -1 (0.00005) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49606 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.32134) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32384 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.14912) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79204 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.61732) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44340 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.26869) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49102 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.31631) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35728 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.18256) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53288 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.35816) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35286 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-1.17814) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47897 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.30425) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69914 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.52442) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80854 HOMO: -6.67767 LUMO: 0.59321 factor:1 | -1 (0.36618) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.66751 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-1.49279) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86902 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.69430) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55620 HOMO: -6.83278 LUMO: 0.39457 factor:1 | -1 (0.61851) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.88280 HOMO: -6.56883 LUMO: 0.64219 factor:1 | -1 (1.29191) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45291 HOMO: -6.71577 LUMO: 0.40001 factor:1 | -1 (0.72181) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.85064 HOMO: -6.86543 LUMO: -0.74287 factor:1 | -1 (1.32408) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55253 HOMO: -6.68584 LUMO: -0.69389 factor:1 | -1 (0.62219) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.89832 HOMO: -6.61237 LUMO: -0.48980 factor:1 | -1 (1.27640) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98525 HOMO: -6.80285 LUMO: -0.58232 factor:1 | -1 (0.18947) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.77650 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.60178) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58442 HOMO: -6.95251 LUMO: -0.71838 factor:1 | -1 (0.59030) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49873 HOMO: -7.52123 LUMO: 0.27211 factor:1 | -1 (0.67599) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53112 HOMO: -6.76747 LUMO: -0.74015 factor:1 | -1 (0.64360) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21682 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.04210) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.05832 HOMO: -6.50896 LUMO: -0.46804 factor:1 | -1 (1.11640) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.06437 HOMO: -7.45320 LUMO: 0.08436 factor:1 | -1 (2.11035) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.24876 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.07404) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46890 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.29418) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72794 HOMO: -6.72665 LUMO: -0.55239 factor:1 | -1 (0.44678) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44085 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.26613) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71651 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (0.45821) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40506 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.23034) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.81828 HOMO: -6.67223 LUMO: -0.45987 factor:1 | -1 (0.35644) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72715 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (0.44757) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20305 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.02833) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07792 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.90320) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94699 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (0.22773) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95936 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.78464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93607 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.76135) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41132 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.23660) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01077 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.16395) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.97028 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (0.20444) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98214 HOMO: -6.66679 LUMO: 0.48708 factor:1 | -1 (0.19257) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59852 HOMO: -6.81917 LUMO: 0.31021 factor:1 | -1 (0.57620) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86189 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.68717) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.24827 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.07355) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99406 HOMO: -7.08857 LUMO: 0.38368 factor:1 | -1 (0.18066) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12489 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.95017) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81821 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-0.64349) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04162 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.86690) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51258 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.33786) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79337 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.61865) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23480 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.06008) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08328 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.90856) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07933 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.90462) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76496 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.59024) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.85915 HOMO: -6.62869 LUMO: -0.24762 factor:1 | -1 (0.31557) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72712 HOMO: -6.65863 LUMO: -0.28028 factor:1 | -1 (0.44760) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01450 HOMO: -6.50352 LUMO: -0.44899 factor:1 | -1 (0.16022) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80015 HOMO: -6.62053 LUMO: -0.88437 factor:1 | -1 (0.37456) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27763 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.10291) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32822 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.15350) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47021 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.29549) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85941 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.68469) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49798 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.32326) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54122 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.36650) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44912 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.27440) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03335 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.85863) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34928 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.17456) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.92383 HOMO: -6.90081 LUMO: 1.82316 factor:1 | -1 (0.25089) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.03541 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (1.13931) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.89570 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (1.27902) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16922 HOMO: -6.11440 LUMO: 1.83949 factor:1 | -1 (0.00550) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59193 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (0.58279) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31951 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.14479) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68970 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.51498) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58988 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.41516) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65175 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.47703) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13000 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.95528) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.62530 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.45058) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.52910 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-2.35438) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.79848 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.62376) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.48001 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (0.69471) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62519 HOMO: -6.50896 LUMO: 2.02725 factor:1 | -1 (0.54953) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57286 HOMO: -6.28583 LUMO: 2.00548 factor:1 | -1 (0.60186) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70633 HOMO: -6.67495 LUMO: 1.92384 factor:1 | -1 (0.46839) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84633 HOMO: -6.17154 LUMO: 2.39732 factor:1 | -1 (0.32839) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02064 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.84592) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.54599 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.37127) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47323 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.29851) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44974 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.27502) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.18491 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-2.01019) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.42770 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.25298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.63921 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.46449) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58778 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-1.41306) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.68538 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-2.51066) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.96300 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.78828) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70970 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (0.46502) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.52679 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (0.64793) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.96760 HOMO: -6.70489 LUMO: 2.20956 factor:1 | -1 (1.20712) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79605 HOMO: -6.94707 LUMO: 1.81500 factor:1 | -1 (0.37867) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62697 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.45225) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48928 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.31456) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.96529 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.79057) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15491 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (0.01981) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23731 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.06259) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97716 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.80244) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.70876 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.53404) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13398 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-0.95926) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.23692 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-1.06220) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05368 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (0.12104) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61788 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.44316) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.99565 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (1.17907) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60891 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (0.56581) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.82503 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (1.34968) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.47520 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (0.69952) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.89810 HOMO: -6.72121 LUMO: 1.33608 factor:1 | -1 (1.27662) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.51341 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.33869) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69331 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-0.51859) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.71339 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (1.46133) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71270 HOMO: -6.78108 LUMO: 2.15786 factor:1 | -1 (0.46202) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.10618 HOMO: -6.50896 LUMO: 2.15786 factor:1 | -1 (1.06854) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75088 HOMO: -6.56067 LUMO: 2.24494 factor:1 | -1 (0.42384) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22325 HOMO: -6.72938 LUMO: 2.24494 factor:1 | -1 (0.95147) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.60438 HOMO: -6.40556 LUMO: 1.58642 factor:1 | -1 (1.57034) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07597 HOMO: -6.63141 LUMO: 1.66262 factor:1 | -1 (0.09875) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.53113 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-0.35641) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.89599 HOMO: -6.86271 LUMO: 1.91296 factor:1 | -1 (0.27873) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75016 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-0.57544) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.88998 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (0.28474) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03828 HOMO: -6.60420 LUMO: 1.79595 factor:1 | -1 (0.13644) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68619 HOMO: -6.85727 LUMO: 2.26943 factor:1 | -1 (0.48853) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57338 HOMO: -6.23413 LUMO: 1.91024 factor:1 | -1 (0.60134) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36660 HOMO: -6.84366 LUMO: 2.01364 factor:1 | -1 (0.80812) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.96558 HOMO: -6.63414 LUMO: 2.54971 factor:1 | -1 (1.20914) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.70710 HOMO: -6.52257 LUMO: 2.42998 factor:1 | -1 (1.46762) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15072 HOMO: -6.61509 LUMO: 2.31297 factor:1 | -1 (0.02400) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39041 HOMO: -6.45998 LUMO: 2.23405 factor:1 | -1 (0.78431) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40752 HOMO: -6.86271 LUMO: 2.22317 factor:1 | -1 (0.76720) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.77624 HOMO: -6.84366 LUMO: 2.11432 factor:1 | -1 (1.39847) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.00466 HOMO: -6.85999 LUMO: 2.44902 factor:1 | -1 (1.17006) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.92484 HOMO: -6.73482 LUMO: 1.93745 factor:1 | -1 (3.24988) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.52410 HOMO: -6.91441 LUMO: 2.32385 factor:1 | -1 (1.65062) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.72120 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (2.45351) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99678 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (0.17794) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55448 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.37976) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22727 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.94745) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49547 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (0.67925) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55612 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.61860) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35688 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.81784) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54486 HOMO: -6.68312 LUMO: 2.30208 factor:1 | -1 (0.62986) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30009 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (0.87463) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.34693 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (1.82779) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75161 HOMO: -6.80829 LUMO: 1.91296 factor:1 | -1 (0.42311) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.10013 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (0.07459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38417 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.20945) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54848 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (0.62624) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63873 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.46401) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22678 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (0.94794) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11706 HOMO: -7.00149 LUMO: 1.80139 factor:1 | -1 (0.05766) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96944 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (0.20528) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35615 HOMO: -6.54434 LUMO: 2.20140 factor:1 | -1 (0.81857) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68576 HOMO: -6.67767 LUMO: 2.02997 factor:1 | -1 (0.48896) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.13599 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (2.03873) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.11438 HOMO: -6.70761 LUMO: 2.71025 factor:1 | -1 (2.06034) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11700 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (0.05772) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94440 HOMO: -6.61781 LUMO: 2.24494 factor:1 | -1 (0.23032) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.82875 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (0.34597) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.90144 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.27328) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28392 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-0.10920) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59947 HOMO: -6.99061 LUMO: 2.13881 factor:1 | -1 (0.57525) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01776 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.84304) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01133 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.83661) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90831 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.73359) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33980 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.16508) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08154 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.90682) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37733 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-1.20261) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03931 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.86459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49153 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-1.31681) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29213 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-1.11741) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57312 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.39840) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45930 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.28458) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21682 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.04210) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08279 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.90807) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87294 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.69822) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83819 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.66347) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.77986 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-2.60514) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.01130 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.83658) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.07021 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.89549) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.63622 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.46150) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58198 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-1.40726) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.25043 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-2.07571) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70989 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-0.53517) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.61841 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-2.44369) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00960 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.16512) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.24812 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-2.07340) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59426 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.41955) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.80490 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.63018) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.22200 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.04728) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63369 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-0.45897) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.39082 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.21610) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46164 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.28692) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81114 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.63642) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86383 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (0.31089) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.99026 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.81554) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.91062 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.73590) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.76852 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.59380) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.74897 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-2.57425) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98328 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-0.80856) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93106 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-0.75634) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.79034 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.61562) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58808 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-1.41336) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61924 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.44452) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87849 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.70377) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.39858 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.22386) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82997 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-0.65525) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21063 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-1.03591) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.18219 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-2.00747) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.30097 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.12625) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.88139 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.70667) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36005 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.18533) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56779 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.39307) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25134 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.07662) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16772 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.99300) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68827 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.51355) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.99995 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.82523) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05425 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-0.87953) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.73623 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.56151) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43621 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.26149) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67674 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.50202) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.17473 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.00001) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.91922 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.74450) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.71431 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.53959) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81737 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.64265) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.82489 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (0.34983) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79403 HOMO: -6.74570 LUMO: 2.20684 factor:1 | -1 (0.38069) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.85202 HOMO: -6.30216 LUMO: 2.15242 factor:1 | -1 (0.32270) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03914 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.86442) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16799 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.99327) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74621 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.57149) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.78981 HOMO: -6.74026 LUMO: 2.21501 factor:1 | -1 (0.38491) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.74886 HOMO: -6.72393 LUMO: 2.19596 factor:1 | -1 (0.42586) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56320 HOMO: -6.11440 LUMO: 2.10072 factor:1 | -1 (0.61152) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44408 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.26936) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24815 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.07343) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.03492 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.86020) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36051 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.18579) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13915 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.96443) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74616 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.57144) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67715 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-0.50243) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21681 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.04209) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.56092 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-1.38620) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28271 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-1.10799) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33889 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.16417) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71528 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (0.45944) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86964 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.69492) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14286 HOMO: -6.78924 LUMO: 2.09256 factor:1 | -1 (0.03186) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.92566 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (1.24906) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.85995 HOMO: -6.75931 LUMO: 1.98643 factor:1 | -1 (1.31477) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65729 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.48257) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.83782 HOMO: -6.83006 LUMO: 1.91840 factor:1 | -1 (0.33690) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.08985 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (0.08487) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05607 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-0.88135) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70931 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.53459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14675 HOMO: -6.85455 LUMO: 2.14970 factor:1 | -1 (0.02797) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43576 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.26104) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25361 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.07889) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85601 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.68129) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40395 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-0.22923) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93306 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (0.24166) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59293 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.41821) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16506 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.00966) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45573 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.28101) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47521 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.30050) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.64456 HOMO: -6.42189 LUMO: 1.99187 factor:1 | -1 (0.53016) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37505 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.20033) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.88212 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (0.29260) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48322 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.30850) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32438 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.14966) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11336 HOMO: -7.05863 LUMO: 2.18780 factor:1 | -1 (0.06136) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69311 HOMO: -6.56611 LUMO: 1.99187 factor:1 | -1 (0.48161) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98677 HOMO: -6.59060 LUMO: 1.86398 factor:1 | -1 (0.18795) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62018 HOMO: -6.59060 LUMO: 1.59459 factor:1 | -1 (0.55454) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.25190 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.92282) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.12964 HOMO: -6.99605 LUMO: 2.30208 factor:1 | -1 (1.04508) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79463 HOMO: -6.42189 LUMO: 2.20412 factor:1 | -1 (0.38009) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.76734 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (0.40738) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.49700 HOMO: -7.08040 LUMO: 2.21773 factor:1 | -1 (1.67772) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26393 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.91079) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68146 HOMO: -6.25590 LUMO: 1.85037 factor:1 | -1 (0.49326) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.13662 HOMO: -6.70489 LUMO: 1.98915 factor:1 | -1 (3.03810) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50991 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.33519) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69800 HOMO: -6.69944 LUMO: 1.98915 factor:1 | -1 (0.47672) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22966 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.05494) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.77066 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (0.40406) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26227 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (0.91245) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.19693 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (0.97779) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89373 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.71901) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.10998 HOMO: -7.19197 LUMO: 2.66127 factor:1 | -1 (0.06474) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60919 HOMO: -6.48175 LUMO: 2.40004 factor:1 | -1 (0.56553) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.76407 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (0.41065) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61836 HOMO: -6.64774 LUMO: 2.13337 factor:1 | -1 (0.55636) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39315 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (0.78157) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.56351 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-1.38879) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.95571 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.78099) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75379 HOMO: -5.87494 LUMO: 2.18235 factor:1 | -1 (0.42093) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.67667 HOMO: -6.30488 LUMO: 2.04902 factor:1 | -1 (0.49805) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.22075 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.04603) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.60726 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.43254) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61377 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.43905) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36451 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.18979) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21126 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.03654) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.74819 HOMO: -6.63414 LUMO: 1.70615 factor:1 | -1 (1.42653) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.88811 HOMO: -7.15115 LUMO: 2.07351 factor:1 | -1 (1.28661) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24233 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-1.06761) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90502 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.73030) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49151 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-1.31679) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53874 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-1.36403) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44500 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-1.27028) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29262 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-1.11790) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46672 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.29201) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02698 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.85226) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37450 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.19978) | -1 | -1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37058 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.19586) | 1 | 1 |
| G: -6121.80903 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.94218 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.76746) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57807 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-0.40335) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18619 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.01147) | 1 | 1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27441 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.09969) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80270 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-0.62798) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49649 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.32177) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20911 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.03440) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.46488 HOMO: -6.83006 LUMO: 0.47348 factor:1 | -1 (0.70984) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.99236 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.81764) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18404 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.00932) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36179 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.18707) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25622 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.08150) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28171 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.10700) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49305 HOMO: -7.34707 LUMO: 0.40001 factor:1 | -1 (0.68167) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.38181 HOMO: -6.19875 LUMO: -0.88709 factor:1 | -1 (0.79291) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57413 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.39941) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33131 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.15659) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.69556 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-2.52084) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.79540 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.62068) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.81984 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.64512) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.82895 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.65423) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13030 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.95558) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.00126 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.82654) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12355 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-0.94883) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.36301 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.18829) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35224 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.17752) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68111 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.50640) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.53710 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.36238) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34282 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.16810) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.23280 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-2.05808) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65398 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.47927) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.59600 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-1.42128) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.29605 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-1.12133) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.38408 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-1.20936) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21536 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.04065) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54756 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.37284) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05224 HOMO: -6.69400 LUMO: -0.07075 factor:1 | -1 (0.12248) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05137 HOMO: -5.28173 LUMO: 1.17281 factor:1 | -1 (0.12335) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62248 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.44776) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.89355 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.71883) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54838 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.37366) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03808 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.86336) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21686 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.04214) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35659 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.18187) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68334 HOMO: -6.47359 LUMO: -0.56600 factor:1 | -1 (0.49138) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.04000 HOMO: -6.63686 LUMO: -0.55783 factor:1 | -1 (1.13471) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.91981 HOMO: -4.13885 LUMO: -2.05446 factor:1 | -1 (1.25491) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68396 HOMO: -6.34570 LUMO: 0.19864 factor:1 | -1 (0.49076) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80739 HOMO: -6.47903 LUMO: 0.24762 factor:1 | -1 (0.36733) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54352 HOMO: -6.15249 LUMO: 0.32109 factor:1 | -1 (0.63120) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02521 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.85049) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19387 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.01915) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16992 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.99520) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97465 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.79993) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06393 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.88921) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76703 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.59231) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.74952 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-1.57480) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98989 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.81517) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.10285 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.92813) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67503 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.50031) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03164 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (0.14308) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94761 HOMO: -6.57155 LUMO: -0.34831 factor:1 | -1 (0.22711) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02693 HOMO: -6.64774 LUMO: -0.95784 factor:1 | -1 (0.14779) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95741 HOMO: -6.91713 LUMO: -0.69933 factor:1 | -1 (0.21731) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98026 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.80554) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.85920 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (0.31552) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92779 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.75308) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02864 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.85392) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66606 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (0.50866) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27700 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-1.10228) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66278 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.48806) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19395 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-1.01923) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20078 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.02606) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93172 HOMO: -6.22052 LUMO: -0.83811 factor:1 | -1 (0.24300) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86018 HOMO: -6.51168 LUMO: -0.76464 factor:1 | -1 (0.31454) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97920 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.80448) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20370 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.02898) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.19565 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.02093) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50070 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-1.32598) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.94977 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-1.77505) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33148 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.15676) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.90022 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.72550) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.31025 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-1.13553) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44179 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.26707) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.72944 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.55472) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.81238 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.63766) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80747 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.63275) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.78627 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.61155) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90246 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.72774) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72105 HOMO: -6.17971 LUMO: 1.67622 factor:1 | -1 (0.45367) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.58000 HOMO: -6.79196 LUMO: 1.36873 factor:1 | -1 (1.59472) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.64539 HOMO: -7.38517 LUMO: 0.56328 factor:1 | -1 (1.52933) | 1 | 1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53196 HOMO: -7.56204 LUMO: 0.71566 factor:1 | -1 (0.64276) | 1 | 1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.76789 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-1.59317) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46512 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.29040) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65064 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.47592) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09770 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.92298) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18969 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.01497) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99920 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.82448) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67718 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.50246) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50221 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.32749) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57590 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-0.40118) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75256 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.42216) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71220 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.53748) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89141 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.71669) | 1 | 1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09570 HOMO: -7.36612 LUMO: 0.63675 factor:1 | -1 (0.07902) | 1 | 1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47919 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.30447) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.51512 HOMO: -6.89264 LUMO: -0.54967 factor:1 | -1 (0.65960) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56618 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.39146) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.66019 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.48547) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67469 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.49997) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93272 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.75800) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05539 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.88067) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58734 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-1.41262) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40531 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.23059) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90442 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.72970) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.08792 HOMO: -6.75659 LUMO: 0.36463 factor:1 | -1 (0.08680) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88483 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.71011) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.96167 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.78695) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.17042 HOMO: -6.91441 LUMO: -1.04492 factor:1 | -1 (0.00430) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85642 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.68170) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84515 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.67043) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53937 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-1.36465) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83057 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67946 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.50474) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.26272 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.08800) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15668 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.01804) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92899 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.75427) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19112 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.01640) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37172 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-1.19700) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31595 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.14123) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11221 HOMO: -6.85183 LUMO: 0.33470 factor:1 | -1 (0.06250) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16585 HOMO: -6.51168 LUMO: 0.48164 factor:1 | -1 (0.00887) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28644 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-1.11172) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67854 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.50382) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29396 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.11924) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21733 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.04261) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54948 HOMO: -6.50624 LUMO: 0.59321 factor:1 | -1 (0.62524) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05050 HOMO: -6.39740 LUMO: 0.83267 factor:1 | -1 (0.12422) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.74105 HOMO: -6.44094 LUMO: 0.65579 factor:1 | -1 (0.43367) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.10672 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (0.06800) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08633 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.91161) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.00377 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.82905) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.73928 HOMO: -6.99333 LUMO: -0.79457 factor:1 | -1 (0.43544) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62512 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.45040) | -1 | -1 |
| G: -6121.80903 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.82570 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.65098) | -1 | -1 |
| G: -6121.80903 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.92182 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.25290) | 1 | 1 |
| G: -6121.80903 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.51332 HOMO: -6.66951 LUMO: 1.34424 factor:1 | -1 (0.66140) | -1 | -1 |
| G: -6121.80903 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.70128 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-1.52656) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44307 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-1.26835) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84945 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.67473) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20745 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-1.03273) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05210 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.87738) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92301 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.74829) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.31733 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.14261) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.15207 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.97735) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34973 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.17501) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.11844 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.94372) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.30707 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.13235) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64414 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.46942) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33158 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.15686) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12540 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.95068) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71065 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.53593) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93522 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.76050) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.49317 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.31845) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93740 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.76268) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05167 HOMO: -6.57155 LUMO: 1.76874 factor:1 | -1 (0.12305) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87692 HOMO: -6.84366 LUMO: 2.04358 factor:1 | -1 (0.29780) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66246 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.48774) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18656 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-0.01184) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.39685 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.22213) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.50273 HOMO: -6.40012 LUMO: 2.17691 factor:1 | -1 (0.67199) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40722 HOMO: -6.80013 LUMO: 2.25582 factor:1 | -1 (0.76750) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28620 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-1.11148) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58936 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.41464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.92140 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.74668) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55805 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.38333) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.96188 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-1.78716) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83372 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.65901) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.07887 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.90415) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.38606 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.21134) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47829 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.30357) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.72689 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.55217) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33485 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.16013) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50783 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-1.33311) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80132 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.62660) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43134 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-1.25662) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.45091 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-1.27619) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.23158 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-1.05686) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18625 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-1.01153) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14437 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.96965) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67301 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-1.49829) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13757 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.96285) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.61627 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.44155) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85177 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.67705) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.71801 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-1.54329) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88257 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.70785) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68016 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-1.50544) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.23096 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-1.05624) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27913 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.10441) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27771 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.10299) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22694 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.05222) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20307 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.02835) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74638 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.57166) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18302 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.00830) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79255 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.61783) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36134 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-0.18662) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02488 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.85017) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.77643 HOMO: -6.85183 LUMO: 1.68711 factor:1 | -1 (0.39829) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56822 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.39350) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15839 HOMO: -6.63141 LUMO: 1.96738 factor:1 | -1 (0.01633) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.10254 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.92782) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34263 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.16791) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33719 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.16247) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01849 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.84377) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72217 HOMO: -6.54978 LUMO: 1.92112 factor:1 | -1 (0.45255) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.64157 HOMO: -6.83006 LUMO: 2.48712 factor:1 | -1 (0.53315) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21405 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.96067) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.15016 HOMO: -6.69944 LUMO: 2.06262 factor:1 | -1 (1.02456) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24621 HOMO: -6.76747 LUMO: 2.10888 factor:1 | -1 (0.92851) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66989 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.49517) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83408 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.65936) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07219 HOMO: -7.03142 LUMO: 2.52250 factor:1 | -1 (0.10253) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62325 HOMO: -6.34025 LUMO: 2.61229 factor:1 | -1 (0.55147) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23059 HOMO: -6.98788 LUMO: 2.28304 factor:1 | -1 (0.94413) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31002 HOMO: -6.97700 LUMO: 2.53882 factor:1 | -1 (0.86470) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20224 HOMO: -6.58788 LUMO: 1.94289 factor:1 | -1 (0.97248) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32672 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.15200) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.39271 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.21799) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97414 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.79942) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99814 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.82342) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09213 HOMO: -6.85727 LUMO: 1.76058 factor:1 | -1 (0.08259) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21490 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.04018) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03650 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.86178) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32791 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.15319) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.37618 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-1.20146) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30207 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.12735) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26807 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.09335) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14872 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.97400) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.80161 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.62689) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06453 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.88981) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32641 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.15169) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94008 HOMO: -6.65046 LUMO: 2.15786 factor:1 | -1 (0.23464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.31561 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.14089) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.90919 HOMO: -6.90081 LUMO: 2.19324 factor:1 | -1 (0.26553) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95893 HOMO: -6.85455 LUMO: 1.95650 factor:1 | -1 (0.21579) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01550 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.84078) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21692 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.04220) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87675 HOMO: -6.97428 LUMO: 1.92929 factor:1 | -1 (0.29796) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.88160 HOMO: -6.61781 LUMO: -0.41906 factor:1 | -1 (0.29312) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43315 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.25843) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71857 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.54385) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71330 HOMO: -6.85727 LUMO: 2.17691 factor:1 | -1 (0.46142) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.99468 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.81996) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03129 HOMO: -7.52395 LUMO: 0.27211 factor:1 | -1 (0.14343) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93787 HOMO: -6.96611 LUMO: -0.72654 factor:1 | -1 (0.23685) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.14613 HOMO: -6.89537 LUMO: -0.68028 factor:1 | -1 (1.02859) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.15908 HOMO: -6.84911 LUMO: -0.58504 factor:1 | -1 (1.01564) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45196 HOMO: -6.79196 LUMO: -0.55783 factor:1 | -1 (0.72276) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.28970 HOMO: -6.67767 LUMO: 1.79323 factor:1 | -1 (0.88502) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59093 HOMO: -6.54434 LUMO: 1.91024 factor:1 | -1 (0.58379) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.50692 HOMO: -6.62869 LUMO: 1.69799 factor:1 | -1 (0.66779) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.48242 HOMO: -6.72393 LUMO: 2.12249 factor:1 | -1 (1.69230) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35014 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.17542) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44233 HOMO: -7.00149 LUMO: 1.82044 factor:1 | -1 (0.73239) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.48684 HOMO: -7.12122 LUMO: 2.16058 factor:1 | -1 (0.68788) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21976 HOMO: -6.63141 LUMO: 2.21229 factor:1 | -1 (0.95496) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.41843 HOMO: -6.37835 LUMO: 2.32113 factor:1 | -1 (0.75629) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31470 HOMO: -6.99605 LUMO: 2.00548 factor:1 | -1 (0.86002) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23350 HOMO: -6.85999 LUMO: 2.39460 factor:1 | -1 (0.94121) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.28967 HOMO: -6.85727 LUMO: 2.48712 factor:1 | -1 (0.88505) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38044 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-0.20572) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30049 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-0.12577) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59389 HOMO: -6.67495 LUMO: 2.14698 factor:1 | -1 (0.58083) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.43974 HOMO: -6.73210 LUMO: 2.06807 factor:1 | -1 (0.73498) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.28975 HOMO: -7.20013 LUMO: 2.02181 factor:1 | -1 (0.88497) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30853 HOMO: -7.18653 LUMO: 2.29936 factor:1 | -1 (0.86619) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30896 HOMO: -6.92802 LUMO: 2.36195 factor:1 | -1 (0.86576) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.19072 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.01600) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.88484 HOMO: -6.96067 LUMO: 2.31297 factor:1 | -1 (0.28988) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.97395 HOMO: -6.91441 LUMO: 2.50345 factor:1 | -1 (0.20077) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20221 HOMO: -7.17292 LUMO: 2.12521 factor:1 | -1 (0.97251) | 1 | 1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.14390 HOMO: -6.93618 LUMO: 2.35106 factor:1 | -1 (1.03082) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.55572 HOMO: -6.75931 LUMO: 1.61908 factor:1 | -1 (1.61900) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.31844 HOMO: -6.35930 LUMO: 1.23540 factor:1 | -1 (1.85628) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36899 HOMO: -6.17971 LUMO: 1.84493 factor:1 | -1 (0.80573) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.46099 HOMO: -6.72665 LUMO: 2.61229 factor:1 | -1 (0.71373) | -1 | -1 |
| G: -6121.80903 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.91154 HOMO: -6.62869 LUMO: 2.28304 factor:1 | -1 (1.26318) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.72234 HOMO: -6.58243 LUMO: 0.28028 factor:1 | -1 (1.45238) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.39496 HOMO: -6.79468 LUMO: 0.14966 factor:1 | -1 (1.77976) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49637 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.67835) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37698 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-0.20226) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30844 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-0.13372) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61463 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (0.56009) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66842 HOMO: -7.19197 LUMO: 1.62996 factor:1 | -1 (0.50630) | 1 | 1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.97931 HOMO: -6.69400 LUMO: 0.84627 factor:1 | -1 (0.19540) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69274 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-0.51802) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79006 HOMO: -6.67767 LUMO: 0.52246 factor:1 | -1 (0.38466) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98865 HOMO: -6.73210 LUMO: 0.94424 factor:1 | -1 (0.18607) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.77931 HOMO: -6.97972 LUMO: 0.60409 factor:1 | -1 (0.39541) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32229 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.14757) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.63414 HOMO: -6.48992 LUMO: 1.08301 factor:1 | -1 (0.54058) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.33631 HOMO: -7.18381 LUMO: 1.61908 factor:1 | -1 (0.83841) | 1 | 1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.77252 HOMO: -6.74842 LUMO: 0.57960 factor:1 | -1 (1.40220) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.32425 HOMO: -6.67495 LUMO: 0.77280 factor:1 | -1 (0.85046) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.65970 HOMO: -6.74570 LUMO: 0.77280 factor:1 | -1 (1.51502) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.43691 HOMO: -6.73754 LUMO: 0.86804 factor:1 | -1 (0.73781) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.80256 HOMO: -6.66135 LUMO: 0.94424 factor:1 | -1 (1.37216) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.80166 HOMO: -6.44638 LUMO: 1.00138 factor:1 | -1 (1.37306) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71416 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.53944) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.41009 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.23537) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.53730 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.36258) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68901 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.51429) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76899 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-0.59427) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61720 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.44248) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50115 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.32643) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70677 HOMO: -6.74298 LUMO: 1.85037 factor:1 | -1 (0.46795) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62238 HOMO: -6.65318 LUMO: 0.95240 factor:1 | -1 (0.55234) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.52891 HOMO: -6.63958 LUMO: 0.78097 factor:1 | -1 (0.64581) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.40503 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-1.23031) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75843 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.58371) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58242 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.40770) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86526 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-0.69054) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13827 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.96356) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86564 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-0.69092) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33033 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.15561) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66243 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.48771) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.81386 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.63914) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63290 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51323 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.33851) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.66909 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.49437) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.43134 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-1.25662) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50503 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.33031) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02799 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.85327) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.80387 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.62915) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.28260 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-1.10788) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55494 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.38022) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.98218 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.80746) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.87364 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.69892) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.71428 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-2.53956) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21534 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.04062) | -1 | -1 |
| G: -6121.80903 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42678 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.25206) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31214 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.13742) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.06104 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (1.11368) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.18520 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (0.98951) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.12126 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (1.05346) | 1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45740 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (0.71732) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.32031 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.85441) | -1 | -1 |
| G: -6121.80903 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61275 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.56197) | 1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49288 HOMO: -7.00149 LUMO: 1.47214 factor:1 | -1 (0.68184) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.29322 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (1.88150) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.45667 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (1.71805) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.16610 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (1.00862) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.48013 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (1.69459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31293 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.86178) | -1 | -1 |
| G: -6121.80903 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.63254 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (1.54218) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.58419 HOMO: -7.00149 LUMO: 1.75241 factor:1 | -1 (1.59053) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29889 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.12417) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52901 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.35429) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55185 HOMO: -6.87360 LUMO: 2.02725 factor:1 | -1 (0.62287) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.81384 HOMO: -7.08584 LUMO: 1.82044 factor:1 | -1 (0.36088) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21858 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.04386) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44649 HOMO: -6.71577 LUMO: 1.93201 factor:1 | -1 (0.72823) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62219 HOMO: -6.99605 LUMO: 2.08439 factor:1 | -1 (0.55253) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.59031 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.41559) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.23324 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.05852) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30321 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.12849) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56526 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.39054) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88303 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.70831) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85130 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.67658) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.11308 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.93836) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.75464 HOMO: -6.88176 LUMO: 2.20684 factor:1 | -1 (1.42008) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.41367 HOMO: -6.73210 LUMO: 2.18780 factor:1 | -1 (0.76105) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.84278 HOMO: -6.83822 LUMO: 2.06807 factor:1 | -1 (1.33194) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43170 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.25698) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42885 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.25413) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.38714 HOMO: -6.85183 LUMO: 1.78779 factor:1 | -1 (0.78758) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.48605 HOMO: -6.98788 LUMO: 1.69799 factor:1 | -1 (0.68867) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56143 HOMO: -6.79468 LUMO: 2.04358 factor:1 | -1 (0.61329) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14729 HOMO: -6.90081 LUMO: 1.97283 factor:1 | -1 (0.02743) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23935 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.06463) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.50698 HOMO: -7.06408 LUMO: 2.29936 factor:1 | -1 (0.66774) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49065 HOMO: -6.78924 LUMO: 2.13337 factor:1 | -1 (0.68407) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63413 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.45941) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70355 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.52883) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33507 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.16035) | -1 | -1 |
| G: -6121.80903 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54179 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.36707) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.73809 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.56337) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.01541 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.84069) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.83170 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.65698) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.05995 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.88523) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.90607 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.73135) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12388.63169 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.45697) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.16119 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.98647) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.17300 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.99828) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25754 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.08282) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27294 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.09822) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.63518 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.46046) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67921 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.50449) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.35295 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.17823) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.38214 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.20742) | 1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36559 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.80913) | 1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30717 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.86755) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06465 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.11007) | 1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11722 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.05750) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.39162 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.21690) | 1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45135 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.27663) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90363 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.72891) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20080 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.97392) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22063 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.95409) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60023 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.57449) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.94593 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (1.22878) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.82871 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.34601) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.37672 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.79800) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20044 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.97428) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11720 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (1.05752) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35650 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.81822) | -1 | -1 |
| G: -6121.80903 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.71717 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (1.45755) | 1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.69896 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (1.47576) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61856 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.44384) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.02488 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.85017) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43124 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.25652) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85321 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.67849) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23494 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.06022) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65720 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.48249) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.90790 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.73318) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.21112 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.03640) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52558 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.35086) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.93269 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.75797) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22027 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.04555) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.24737 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.07265) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.64039 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.46567) | 1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46330 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.28858) | 1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.32064 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.85408) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26488 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.90984) | 1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59503 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.42031) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85226 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.67754) | 1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.83187 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.65715) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.81948 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.64477) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68737 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.51265) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57933 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.40461) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04869 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.87398) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38811 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.21339) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.97768 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.19704) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28280 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.10808) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61427 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.56045) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.17942 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.00470) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98821 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.18651) | -1 | -1 |
| G: -6121.80903 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65451 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.47979) | 1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26807 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.09335) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41467 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.23995) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13272 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.95800) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.19956 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.02484) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.60919 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.43448) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52305 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.34833) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.65894 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.48422) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76140 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.58668) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.77294 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.40178) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66270 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.48798) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12394 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.05078) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09830 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.92358) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.08034 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.90562) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58417 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.40945) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03993 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.86521) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24992 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.07520) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33180 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.15708) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03259 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.14213) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74834 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.57362) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.72278 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.54806) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36770 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.19298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.67176 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.49704) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.64295 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.53176) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83658 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.66186) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93531 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.23941) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.72914 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.55442) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.97784 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.80312) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.42791 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.25319) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86567 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.69095) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.17591 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.00119) | -1 | -1 |
| G: -6121.80903 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.18157 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.00685) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06228 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.11244) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84260 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.33211) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27357 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.09885) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.86190 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.31282) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01129 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.16343) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94405 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.23067) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15850 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.01622) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99333 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.18139) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61699 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.55772) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56184 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.61288) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.28248 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.10776) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22517 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.05045) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11500 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.05972) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71281 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.46191) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59078 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.41606) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.55377 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.37905) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13036 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.04435) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.05577 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.88105) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84880 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.67408) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34903 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.17431) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69868 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.47604) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58742 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.58730) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36464 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.81008) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25497 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.08025) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.19333 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.01861) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.03029 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.14443) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44339 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.73133) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36744 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.80728) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07853 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.09619) | -1 | -1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01719 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.15753) | 1 | 1 |
| G: -6121.80903 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.91935 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (1.25537) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58320 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.59152) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99180 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.18291) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02435 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.15037) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.74682 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.42790) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70402 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.47070) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.76535 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.40937) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70867 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.46605) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.85763 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.31709) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37301 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.19829) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62210 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.44738) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95708 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.21764) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69138 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.51666) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59214 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.41742) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79855 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.37617) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44395 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.26923) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58243 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.40771) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38651 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.21179) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49203 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.31731) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02236 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.15236) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.72119 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.45353) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23435 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.94037) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57958 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.59514) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53650 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.63822) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21812 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.04340) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.13431 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.04041) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.08311 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.09161) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.67411 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.50061) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.65569 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.51903) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.01589 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.15883) | -1 | -1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09581 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.07891) | 1 | 1 |
| G: -6121.80903 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71582 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.54110) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66235 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.48763) | 1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95512 HOMO: -5.10213 LUMO: 0.77825 factor:1 | -1 (0.21960) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87534 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.29938) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99167 HOMO: -5.39874 LUMO: 0.68028 factor:1 | -1 (0.18305) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.94878 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (0.22594) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.58790 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.41318) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.54186 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-0.36714) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12343 HOMO: -5.80963 LUMO: 0.56328 factor:1 | -1 (0.05129) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40583 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-0.23111) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43595 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-0.26123) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69318 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-0.51846) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.40482 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-0.23010) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.64791 HOMO: -5.86405 LUMO: 0.55511 factor:1 | -1 (0.52681) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.83417 HOMO: -5.64908 LUMO: 0.71022 factor:1 | -1 (0.34055) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09502 HOMO: -5.94297 LUMO: 0.68301 factor:1 | -1 (0.07970) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14936 HOMO: -6.01916 LUMO: 0.56328 factor:1 | -1 (0.02536) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.16433 HOMO: -6.05181 LUMO: 0.35103 factor:1 | -1 (1.01039) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49324 HOMO: -6.08447 LUMO: 0.48436 factor:1 | -1 (0.68148) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45008 HOMO: -5.86950 LUMO: 0.36735 factor:1 | -1 (0.72464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11839 HOMO: -5.33615 LUMO: 0.65852 factor:1 | -1 (0.05633) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.10019 HOMO: -5.36064 LUMO: 0.86804 factor:1 | -1 (0.07453) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.98422 HOMO: -5.74160 LUMO: 0.64491 factor:1 | -1 (1.19050) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60880 HOMO: -5.23003 LUMO: 0.66124 factor:1 | -1 (0.56592) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.53493 HOMO: -5.77698 LUMO: 0.84083 factor:1 | -1 (0.63979) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06177 HOMO: -5.60555 LUMO: 0.84355 factor:1 | -1 (0.11295) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25238 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-0.07766) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.68300 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.50828) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79658 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.62186) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.40907 HOMO: -6.99333 LUMO: -0.88709 factor:1 | -1 (0.76565) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.50118 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.67354) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.33842 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-0.16370) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31712 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-0.14240) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.58109 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.40637) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48191 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-0.30719) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04059 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-0.86587) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.32604 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-0.15132) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00223 HOMO: -7.07224 LUMO: -1.89391 factor:1 | -1 (0.17249) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29548 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-0.12076) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.10392 HOMO: -7.24367 LUMO: 0.29388 factor:1 | -1 (1.07080) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.03622 HOMO: -7.02326 LUMO: -0.87893 factor:1 | -1 (1.13850) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.71577 HOMO: -6.88176 LUMO: 0.71566 factor:1 | -1 (0.45895) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59680 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.42208) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54873 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.37401) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12234 HOMO: -6.73210 LUMO: -1.06941 factor:1 | -1 (0.05238) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06437 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-0.88965) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79996 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-0.62524) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27920 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.10448) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61343 HOMO: -7.34163 LUMO: 0.35103 factor:1 | -1 (0.56129) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45846 HOMO: -6.87632 LUMO: -0.87349 factor:1 | -1 (0.71626) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24529 HOMO: -7.06952 LUMO: -1.47214 factor:1 | -1 (0.92943) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12808 HOMO: -6.58788 LUMO: -0.37824 factor:1 | -1 (0.04664) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.07793 HOMO: -6.92802 LUMO: -1.24900 factor:1 | -1 (0.09679) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.91426 HOMO: -7.01237 LUMO: -1.31975 factor:1 | -1 (1.26046) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13098 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.95626) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67058 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.49586) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74942 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-0.57470) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37309 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.19837) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04527 HOMO: -7.21646 LUMO: 0.13061 factor:1 | -1 (0.12944) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.02547 HOMO: -6.62597 LUMO: -0.64763 factor:1 | -1 (0.14925) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66472 HOMO: -7.38789 LUMO: 0.31021 factor:1 | -1 (0.51000) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68521 HOMO: -6.74570 LUMO: -0.70750 factor:1 | -1 (0.48951) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58154 HOMO: -6.95251 LUMO: -1.25989 factor:1 | -1 (0.59318) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55767 HOMO: -7.13483 LUMO: -0.76736 factor:1 | -1 (0.61705) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55906 HOMO: -6.93618 LUMO: -1.24628 factor:1 | -1 (0.61566) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04413 HOMO: -7.03686 LUMO: 0.26395 factor:1 | -1 (0.13059) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16060 HOMO: -6.52257 LUMO: -0.84355 factor:1 | -1 (0.01412) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93025 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.24447) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.55690 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-0.38218) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.25445 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-0.07973) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58782 HOMO: -7.09401 LUMO: -0.92519 factor:1 | -1 (0.58690) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47364 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.29892) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.31540 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.14068) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49021 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.31549) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.97733 HOMO: -6.20964 LUMO: 0.99866 factor:1 | -1 (0.19739) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.62682 HOMO: -6.52801 LUMO: 1.07757 factor:1 | -1 (0.54790) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21897 HOMO: -6.74298 LUMO: -0.67756 factor:1 | -1 (0.95575) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.27193 HOMO: -7.43959 LUMO: 0.03265 factor:1 | -1 (0.90279) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.22613 HOMO: -6.46815 LUMO: -0.29933 factor:1 | -1 (0.94859) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.82807 HOMO: -6.70489 LUMO: -0.97145 factor:1 | -1 (0.34665) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.78666 HOMO: -6.30216 LUMO: -1.39322 factor:1 | -1 (0.38806) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.76419 HOMO: -7.01782 LUMO: -1.07485 factor:1 | -1 (1.41053) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80911 HOMO: -6.93074 LUMO: 0.25851 factor:1 | -1 (0.36561) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26529 HOMO: -7.07224 LUMO: 0.09524 factor:1 | -1 (0.90943) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49026 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.31554) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36781 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.19309) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.54079 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.36607) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37851 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-0.20379) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.83465 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.65993) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66931 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.49459) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41584 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-0.24112) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.49805 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.32333) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23858 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.06387) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09551 HOMO: -6.57699 LUMO: -1.14016 factor:1 | -1 (0.07921) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.83006 HOMO: -6.57699 LUMO: -1.31975 factor:1 | -1 (0.34466) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.67803 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.49669) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36641 HOMO: -7.25728 LUMO: 0.29660 factor:1 | -1 (0.80831) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21998 HOMO: -6.37019 LUMO: -0.95240 factor:1 | -1 (0.95474) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.18956 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (0.98516) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68524 HOMO: -6.37291 LUMO: -0.78641 factor:1 | -1 (0.48948) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.64587 HOMO: -6.65863 LUMO: -0.69933 factor:1 | -1 (0.52885) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.42314 HOMO: -6.44638 LUMO: -0.16055 factor:1 | -1 (0.75158) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30279 HOMO: -6.41917 LUMO: -0.20136 factor:1 | -1 (0.87193) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60799 HOMO: -7.33347 LUMO: 0.12789 factor:1 | -1 (0.56673) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57784 HOMO: -6.70489 LUMO: -0.52518 factor:1 | -1 (0.59688) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49215 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.68257) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26580 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.90891) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44175 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.73297) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.70603 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (0.46869) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.75319 HOMO: -6.24501 LUMO: -0.44627 factor:1 | -1 (0.42153) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.45944 HOMO: -6.73754 LUMO: -0.45443 factor:1 | -1 (0.71528) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.14493 HOMO: -6.24501 LUMO: 0.38096 factor:1 | -1 (1.02979) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.17247 HOMO: -6.86815 LUMO: -0.91974 factor:1 | -1 (1.00225) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.84878 HOMO: -7.40150 LUMO: 0.36191 factor:1 | -1 (0.32594) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.76511 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.40961) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.71684 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (1.45788) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.92971 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.24501) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45184 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.27712) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.35706 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.18234) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.69814 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (0.47658) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.20131 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.97341) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.90105 HOMO: -6.75659 LUMO: -0.68845 factor:1 | -1 (0.27366) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.92497 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.24975) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.68426 HOMO: -6.28583 LUMO: -0.46804 factor:1 | -1 (0.49046) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66989 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (0.50483) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16666 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.00805) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93700 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.23772) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.05896 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (0.11576) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21418 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.03946) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.66227 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.51244) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96394 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.21078) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41932 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.24460) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.99325 HOMO: -5.90759 LUMO: 2.00820 factor:1 | -1 (0.18147) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.08683 HOMO: -6.56339 LUMO: 1.99732 factor:1 | -1 (0.08789) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.96021 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.21451) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80345 HOMO: -6.16882 LUMO: 1.94017 factor:1 | -1 (0.37127) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41600 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.24128) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15502 HOMO: -6.58243 LUMO: 1.78235 factor:1 | -1 (0.01970) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42316 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.24844) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21404 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.03932) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.52814 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.35342) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.15994 HOMO: -7.06135 LUMO: 0.29660 factor:1 | -1 (0.01478) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79376 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (0.38096) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98688 HOMO: -6.68040 LUMO: -0.60681 factor:1 | -1 (0.18784) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.34012 HOMO: -6.93618 LUMO: -1.09662 factor:1 | -1 (0.83460) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.37490 HOMO: -6.72121 LUMO: -1.14016 factor:1 | -1 (0.79982) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31998 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (0.85474) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59740 HOMO: -6.71305 LUMO: -0.71566 factor:1 | -1 (0.57732) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00174 HOMO: -7.09401 LUMO: -0.86532 factor:1 | -1 (0.17298) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.56301 HOMO: -7.08584 LUMO: -0.92519 factor:1 | -1 (0.61171) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.29374 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-0.11902) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27165 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-0.09693) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54244 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (0.63228) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00759 HOMO: -6.81373 LUMO: -1.72248 factor:1 | -1 (0.16713) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.14432 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (0.03040) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09281 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (0.08191) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03382 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (0.14090) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.59680 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (0.57792) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.32679 HOMO: -7.04231 LUMO: -0.83539 factor:1 | -1 (0.84793) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.87823 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (1.29649) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.21593 HOMO: -6.89809 LUMO: -1.19186 factor:1 | -1 (0.95879) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.14782 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (1.02690) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.90824 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (0.26648) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.80650 HOMO: -6.84366 LUMO: -0.88437 factor:1 | -1 (0.36822) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.69260 HOMO: -6.91986 LUMO: -1.12655 factor:1 | -1 (1.48212) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.90895 HOMO: -6.49536 LUMO: -0.29660 factor:1 | -1 (0.26577) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.65716 HOMO: -6.74842 LUMO: 0.42450 factor:1 | -1 (0.51756) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.91934 HOMO: -7.34435 LUMO: 0.32109 factor:1 | -1 (0.25538) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.55256 HOMO: -7.16476 LUMO: 0.28572 factor:1 | -1 (0.62216) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87673 HOMO: -6.74298 LUMO: -0.43538 factor:1 | -1 (0.29799) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.79161 HOMO: -7.19469 LUMO: -1.61091 factor:1 | -1 (0.38311) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.37353 HOMO: -7.35252 LUMO: -1.78235 factor:1 | -1 (0.80118) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.78660 HOMO: -7.25456 LUMO: -1.66806 factor:1 | -1 (0.38812) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03948 HOMO: -7.54844 LUMO: -1.07213 factor:1 | -1 (0.13524) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.68654 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (2.48818) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.77180 HOMO: -7.01782 LUMO: -1.60547 factor:1 | -1 (0.40292) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34003 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.16531) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27252 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-0.09780) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.38251 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.20779) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.12988 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (0.04484) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22375 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-0.04903) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23341 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-0.05869) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.20803 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.03331) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59497 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.42025) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.56297 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.38825) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50654 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.33182) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41413 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.23941) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.46738 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.29266) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.41356 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.76116) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.33255 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.84217) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06375 HOMO: -7.07224 LUMO: 0.85988 factor:1 | -1 (0.11097) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.00525 HOMO: -7.02326 LUMO: 1.10206 factor:1 | -1 (0.16947) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.88909 HOMO: -6.71305 LUMO: 0.84627 factor:1 | -1 (1.28563) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09926 HOMO: -7.27360 LUMO: 0.88165 factor:1 | -1 (0.07546) | 1 | 1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41037 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.23565) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41551 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-0.24079) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.60603 HOMO: -6.97156 LUMO: 0.53606 factor:1 | -1 (0.56869) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.25927 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.91545) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.49944 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (0.67528) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.04612 HOMO: -6.34025 LUMO: 0.50341 factor:1 | -1 (0.12860) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.93390 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (0.24082) | -1 | -1 |
| G: -6121.80903 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22585 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-0.05113) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29623 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-1.16693) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43398 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.30468) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35999 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.23069) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20328 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.07398) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47825 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.34895) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06608 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.93678) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68575 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.55645) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54950 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.42020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39126 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-0.26196) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50727 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-0.37797) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53921 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.40991) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37306 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-0.24376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32587 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-0.19658) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61535 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-0.48605) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46498 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-0.33568) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40590 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-0.27660) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30987 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.18057) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47763 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.34833) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36111 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.23181) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06717 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.93787) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83263 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.70333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86730 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.73800) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10483 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.97553) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07065 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.94135) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27060 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-1.14130) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99666 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.86736) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48835 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.35905) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18467 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-1.05537) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85802 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-0.72872) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84545 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.71615) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79552 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.66622) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15394 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-1.02464) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14113 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-1.01183) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36524 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-1.23594) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44062 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.31132) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43428 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.30498) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27406 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.14476) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28034 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.15104) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12896 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-0.99966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28162 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.15232) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05473 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-0.92543) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20230 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.07300) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02684 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-0.89754) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97092 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-0.84162) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14526 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.01596) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28684 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.15755) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42557 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.29627) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20638 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.07708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32263 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.19333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49580 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.36650) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36102 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-1.23172) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25188 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-1.12258) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31898 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.18968) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56889 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-1.43959) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37517 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-1.24587) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41248 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.28318) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49264 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-1.36334) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55281 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.42351) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42462 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.29532) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30187 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-1.17257) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30080 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-1.17150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06046 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.93116) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82794 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.69864) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01655 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.88725) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31963 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-2.19033) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17432 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-2.04502) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88207 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.75277) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95361 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.82431) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96405 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.83475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.27081 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-2.14151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06955 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.94025) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84307 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.71377) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74789 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.61859) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05042 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-1.92112) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02000 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-1.89070) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86664 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-1.73734) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07851 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.94921) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93252 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.80322) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21614 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-2.08684) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09970 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.97040) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10705 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-1.97775) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98822 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-1.85892) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91858 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-1.78928) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09018 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-1.96088) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93975 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-1.81046) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97374 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.84444) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07826 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.94896) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01246 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.88316) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93633 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.80703) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21927 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.08997) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86773 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-1.73843) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90144 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.77214) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34807 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-1.21877) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29346 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-1.16416) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25362 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-1.12432) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44614 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.31684) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39079 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-1.26149) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28671 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-1.15741) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27621 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.14691) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25803 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.12873) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90958 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.78028) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20254 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-2.07324) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35707 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-2.22777) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51993 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-2.39063) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09361 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-1.96431) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53463 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.40533) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03903 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.90973) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96548 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.83618) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23288 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.10358) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92062 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-2.79132) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03502 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.90572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32847 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-2.19917) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.39462 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-2.26532) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11671 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.98741) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06163 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.93233) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08602 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.95672) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.43057 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-2.30127) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30169 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-2.17239) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31190 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-2.18260) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.20070 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-3.07140) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36695 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-2.23765) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19764 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-2.06834) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17119 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-2.04189) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.91172 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-2.78242) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61817 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-1.48887) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45991 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-1.33061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50807 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-1.37877) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37789 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-1.24859) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15573 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-2.02643) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53697 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-1.40767) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36668 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.23738) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35838 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-1.22908) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32336 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-1.19406) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10131 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-1.97201) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.52695 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-2.39765) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30064 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-1.17134) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31751 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-1.18821) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16135 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-1.03205) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35664 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-1.22734) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90983 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.78053) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.99063 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-2.86133) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.13692 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-3.00762) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80533 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-1.67603) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95502 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-1.82572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74072 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-2.61142) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16893 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-2.03963) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26833 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-2.13903) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19043 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-2.06113) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75939 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-2.63009) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50812 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-2.37882) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80573 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-2.67643) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28583 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-2.15653) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25601 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-2.12671) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24939 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-2.12009) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13437 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-2.00507) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91284 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.78354) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.73280 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-2.60350) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.64145 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-2.51216) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63661 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-2.50731) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.95956 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-2.83026) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08934 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-1.96004) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89009 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.76079) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13758 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-2.00828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.82712 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-2.69782) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01475 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-1.88545) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22338 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-2.09408) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72573 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-2.59643) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.68916 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-2.55986) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59593 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-2.46663) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.49736 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-3.36806) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09832 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-1.96902) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01203 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-1.88273) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72348 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.59418) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.70769 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-2.57839) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03306 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-1.90376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84552 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-1.71622) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84256 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-1.71326) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67819 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-2.54889) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.32294 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-3.19364) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91094 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-1.78164) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75855 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-1.62925) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59096 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-1.46166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61773 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-2.48843) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92225 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-2.79295) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09815 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-1.96885) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03486 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-1.90556) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98003 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-1.85073) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69621 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-1.56691) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15775 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-2.02845) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78731 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-2.65801) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84496 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.71566) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34624 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-2.21694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61194 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-1.48264) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79455 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-1.66526) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.09820 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (0.03110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67649 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.54719) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52642 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.39712) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91473 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.78543) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90416 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.77486) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.70597 HOMO: -6.58788 LUMO: -1.03947 factor:1 | -1 (0.42333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32898 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.19968) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90984 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-2.78054) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21881 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-2.08951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45806 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-1.32876) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84781 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-1.71851) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80523 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.67593) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63075 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.50145) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.76619 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-2.63689) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93641 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-1.80711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19418 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-2.06488) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93415 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-1.80485) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.64091 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-2.51161) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66191 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.53261) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49113 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.36183) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78776 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.65846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63730 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.50800) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59164 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-1.46234) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68459 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.55529) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66691 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-1.53761) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39792 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-1.26862) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75684 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-1.62754) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54560 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.41630) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44334 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-1.31404) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65167 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-1.52237) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45294 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-1.32364) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11508 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-1.98578) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60595 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-1.47665) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40289 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-2.27359) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50907 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-2.37977) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07027 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.94097) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.84783 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-2.71853) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92789 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-1.79859) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06738 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.93808) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12667 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-1.99737) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15192 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-2.02262) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94971 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.82041) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21429 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-2.08499) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85491 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.72561) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76190 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.63260) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07399 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.94469) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.18021 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-3.05091) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85363 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.72433) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.54875 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-2.41945) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01902 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.88972) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88064 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-2.75134) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95095 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.82165) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98880 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.85950) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47609 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-2.34679) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59253 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-2.46323) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70354 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.57424) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80275 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.67345) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93688 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.80758) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63222 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.50292) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87323 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.74393) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.84154 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-2.71224) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41702 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.28772) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61205 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.48275) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44034 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-2.31104) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.92198 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.20732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.60575 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.52355) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14753 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-0.01823) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38495 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-0.25565) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37679 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.24749) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70077 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-0.57147) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.97768 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-2.84838) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16517 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-2.03587) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11325 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.98395) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73649 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.60719) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80770 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-1.67840) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81156 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.68226) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70512 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.57582) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66248 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.53318) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59178 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-0.46248) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82082 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.69152) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09954 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-1.97024) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.73814 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-2.60884) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02980 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.90050) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07747 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.94817) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15788 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-2.02858) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91265 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.78335) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06534 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.93604) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97056 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-1.84126) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00305 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.87375) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61644 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.48714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65464 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.52534) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65677 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.52747) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74770 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.61840) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83382 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-1.70452) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95165 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-1.82235) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05943 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.93013) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56726 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.43796) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63091 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.50161) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67398 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-1.54468) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45844 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-1.32914) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79115 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-1.66185) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28917 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.15987) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45986 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-0.33056) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.18350 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-0.05421) | 1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28528 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-0.15598) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.03079 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.09851) | 1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22706 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.09776) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04888 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.91958) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26050 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-1.13120) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64675 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.51745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79405 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.66475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72694 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.59764) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86531 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.73601) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14170 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-1.01240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93097 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.80167) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86510 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.73580) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74583 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.61653) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84335 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-0.71405) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95476 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-0.82546) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85788 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-0.72858) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62476 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-0.49546) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92926 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-0.79996) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23678 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.10748) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49605 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-1.36675) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47501 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.34571) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48021 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-1.35091) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37096 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-1.24166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78432 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-1.65502) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47227 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-0.34297) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62909 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-0.49979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78907 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-0.65977) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50759 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.37829) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69815 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-0.56885) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69519 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.56589) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85772 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.72842) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76564 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.63634) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96302 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.83372) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95023 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.82093) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05355 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.92425) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00588 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.87658) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11943 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.99013) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96354 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.83424) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84930 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-1.72000) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85548 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.72618) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68908 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.55978) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67170 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-1.54240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.93289 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-2.80359) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08515 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.95585) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14705 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-2.01775) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81470 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-0.68540) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51818 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-0.38888) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.98190 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.14740) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.22745 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-0.09815) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.80886 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.32044) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08595 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.04335) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.75678 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (0.37252) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91704 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-0.78774) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08159 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-0.95229) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73698 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-0.60768) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81029 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.68099) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67837 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-0.54907) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44234 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-0.31304) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73924 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-0.60994) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62751 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-0.49821) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54351 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-0.41421) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16064 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-1.03134) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26875 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-1.13945) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38203 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-1.25273) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00074 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-1.87144) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01415 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-1.88485) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.93803 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-2.80873) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09641 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.96711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09138 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.96208) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14939 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-2.02009) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24678 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-2.11748) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02335 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-1.89405) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01173 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-1.88243) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70353 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-1.57423) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74040 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.61110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86843 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-1.73913) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93722 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.80792) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90427 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.77497) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65494 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-0.52564) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75168 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.62238) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60955 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.48025) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98298 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-0.85368) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97774 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-1.84844) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17075 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-2.04145) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66806 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.53876) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67943 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.55013) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74107 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.61177) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14477 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-2.01547) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65561 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.52631) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64467 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.51537) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90512 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.77582) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75693 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.62763) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75674 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.62744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95862 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.82932) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86735 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.73805) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51986 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.39057) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67130 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.54200) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46952 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.34022) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56795 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.43865) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82569 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.69639) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91718 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-0.78788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65589 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.52659) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13808 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.00878) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09441 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.96511) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37150 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-1.24220) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49509 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-1.36579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61273 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-1.48343) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69902 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-0.56972) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66936 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.54006) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65818 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.52888) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77426 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-0.64496) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03706 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.90776) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59881 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-2.46951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.44561 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-3.31631) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.35646 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-3.22716) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.82742 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-2.69812) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06041 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-1.93111) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68817 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-0.55887) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89337 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-0.76407) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72825 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.59895) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76245 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-0.63315) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45863 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.32933) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61624 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-1.48694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67711 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.54781) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45985 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.33056) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64304 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-1.51374) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27033 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.14103) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53221 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.40291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03902 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-1.90972) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98444 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.85514) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.34971 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-3.22041) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48741 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-2.35811) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.60839 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-2.47909) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86228 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-2.73298) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76223 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.63293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91048 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.78118) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09443 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-0.96513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.09281 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-2.96351) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76726 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.63796) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.83863 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-2.70933) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23026 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-2.10096) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86462 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-2.73532) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86844 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-0.73914) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93677 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.80747) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50208 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.37278) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68846 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.55916) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67882 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-1.54953) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89192 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-1.76262) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.96426 HOMO: -6.60692 LUMO: -0.47076 factor:1 | -1 (0.16504) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28168 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.15238) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66817 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.53887) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49728 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.36798) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89663 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-0.76733) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79983 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.67053) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.71580 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (0.41350) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.70360 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (0.42569) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.19504 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.06574) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40911 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-0.27981) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90266 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-2.77336) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02294 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.89364) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10316 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-1.97386) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63330 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.50400) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64408 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-1.51478) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76119 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.63189) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49456 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-0.36526) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63649 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.50719) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60425 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-0.47495) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.76314 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-2.63384) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88767 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.75837) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94691 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-1.81761) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13179 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-2.00249) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97015 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-1.84085) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94503 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.81573) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67588 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-2.54658) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60528 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.47598) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79810 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.66880) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63641 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-0.50711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49573 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-0.36643) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70188 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.57258) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66057 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-0.53128) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52498 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.39568) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72177 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-0.59247) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81881 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-0.68951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73067 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.60137) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55170 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.42240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66558 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.53628) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69652 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.56722) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72879 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.59949) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67892 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.54962) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59078 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.46148) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41434 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.28504) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65483 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-0.52553) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52079 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.39149) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71062 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.58132) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89807 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.76877) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06395 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.93465) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06495 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-1.93565) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05505 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-1.92575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96180 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.83250) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81080 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-1.68150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45038 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-2.32108) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90247 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-2.77317) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62024 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-1.49094) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49556 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-1.36626) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58424 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-1.45494) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67314 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-1.54384) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85254 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-1.72324) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69564 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.56634) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77766 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.64836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74816 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-1.61886) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44244 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.31314) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77600 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.64670) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75210 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.62281) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70552 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-1.57622) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67453 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-1.54523) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81488 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.68558) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74767 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-1.61837) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78032 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-1.65102) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72304 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-1.59374) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87486 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.74556) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81480 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.68550) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70517 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-1.57587) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59793 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-1.46863) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61744 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.48814) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73254 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-1.60324) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34695 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-2.21765) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18727 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-2.05797) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47065 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-2.34135) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06575 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.93645) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89076 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-0.76146) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.25847 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-3.12917) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94375 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.81446) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93042 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.80112) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74135 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-2.61205) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.58891 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-2.45961) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70100 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.57170) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61553 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.48623) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52995 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.40065) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72830 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.59900) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99660 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.86730) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85437 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.72507) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73502 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.60572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52465 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.39535) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36547 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-0.23617) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53616 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.40686) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60041 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.47111) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51811 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.38881) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74868 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-1.61938) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46388 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.33458) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68356 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.55426) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59931 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-1.47001) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40170 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.27240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57665 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.44735) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72710 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.59780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47402 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-2.34472) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67929 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.54999) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57550 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.44620) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30281 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-2.17351) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63420 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.50490) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58448 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.45518) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69259 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.56329) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.27367 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-2.14437) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63809 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.50879) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63961 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.51031) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44867 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.31937) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32101 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-2.19171) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63855 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.50925) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88489 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-2.75559) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26376 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-2.13446) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50650 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.37720) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44239 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.31309) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59401 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-1.46471) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90603 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-2.77673) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51275 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-1.38345) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41866 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.28936) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42165 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.29235) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69477 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-1.56547) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81983 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-2.69053) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52043 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.39113) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14104 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-2.01174) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39732 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.26802) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61036 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.48106) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48776 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-2.35847) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50910 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-2.37980) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86691 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-1.73761) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72498 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.59568) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83827 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.70897) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96063 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.83134) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82471 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.69541) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88314 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.75384) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66063 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.53133) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.76682 HOMO: -6.53073 LUMO: 1.73337 factor:1 | -1 (0.36248) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.06546 HOMO: -5.91303 LUMO: 1.90480 factor:1 | -1 (0.06384) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12235 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.99305) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23931 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.11001) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40315 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.27385) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46932 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.34002) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43942 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.31012) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78444 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.65514) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03457 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.90527) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75472 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.62542) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95053 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.82123) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05709 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.92779) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45183 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-1.32253) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34383 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.21453) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39248 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.26318) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64601 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-1.51671) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52481 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.39551) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53558 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.40628) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40902 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.27972) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39925 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-1.26996) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06787 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.93858) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27795 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.14865) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41613 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.28683) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20387 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-2.07457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.10443 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-2.97513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21897 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-2.08967) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26069 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-2.13139) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44537 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-2.31607) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13304 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-2.00374) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10640 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.97710) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03042 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.90112) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97744 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.84814) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99658 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.86728) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88510 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.75580) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.39696 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-2.26766) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96582 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.83652) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83817 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.70888) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82991 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-0.70061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88286 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-0.75356) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70811 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.57881) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85437 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-0.72507) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30324 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-2.17394) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71727 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.58797) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92803 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.79873) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75798 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-1.62868) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42271 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-1.29341) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65836 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-1.52906) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55569 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-1.42639) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42105 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.29175) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99340 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.86410) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05421 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-0.92492) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77739 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.64809) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78414 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-0.65484) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90686 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.77757) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81285 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.68355) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79603 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.66673) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64670 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-0.51740) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89037 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.76108) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69113 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.56183) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50539 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.37609) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20605 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-2.07675) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45760 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.32830) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88280 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.75350) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69624 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.56694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91941 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-0.79011) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11998 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.99068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97560 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.84630) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04621 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.91691) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06475 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.93545) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05424 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.92494) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08872 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.95942) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86474 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-0.73544) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40758 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.27828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46296 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.33366) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85429 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.72499) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09084 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.96154) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07381 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.94451) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16603 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.03673) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06885 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-0.93955) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89873 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-0.76943) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15372 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-2.02442) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08487 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-1.95557) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14683 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-2.01753) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31908 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-2.18978) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00201 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.87271) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04860 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.91930) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13187 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-2.00257) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11413 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.98483) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66206 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.53276) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87845 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.74915) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64555 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.51625) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60456 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.47527) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79094 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.66164) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70413 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.57483) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67061 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.54131) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61205 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.48275) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63648 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.50718) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89292 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.76362) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62518 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-2.49588) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.22723 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-3.09793) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.97836 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-2.84906) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47587 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-2.34657) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.54619 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-2.41689) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.33873 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-2.20943) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.58690 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-2.45760) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86476 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.73546) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66190 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.53260) | 1 | 1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80881 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.67951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91137 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.78207) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76420 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.63490) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03451 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-0.90521) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77266 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-0.64336) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95536 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-0.82606) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83225 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.70295) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05438 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-0.92508) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68882 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.55952) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78909 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.65979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87767 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.74837) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84662 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.71732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40224 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-2.27294) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68375 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-1.55445) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75864 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-1.62934) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85676 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.72746) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57099 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.44169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72865 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-1.59935) | -1 | -1 |
| G: -5278.76361 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71439 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.58509) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49752 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.36822) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42981 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.30051) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57967 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.45037) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28118 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-1.15189) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53678 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-1.40748) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17716 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.04786) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56565 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.43635) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84060 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.71130) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42287 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-1.29357) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51733 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-1.38803) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60397 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-1.47467) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54045 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-1.41116) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72402 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-1.59472) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69668 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-1.56738) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57139 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-1.44209) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73597 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-1.60667) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75038 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-2.62108) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.43352 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-3.30422) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.22658 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-3.09728) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.53710 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-2.40780) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.99308 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-2.86378) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36853 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-1.23923) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55177 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-1.42248) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52881 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-1.39951) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55341 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.42411) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49545 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-1.36615) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39762 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.26832) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20275 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-2.07345) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20811 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-2.07881) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42646 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-2.29716) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47302 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-2.34372) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48301 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.35371) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57529 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.44599) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46209 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.33279) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80484 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.67554) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43324 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.30394) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51074 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-1.38144) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69311 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-1.56381) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.20114 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-3.07184) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47835 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-2.34905) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62067 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-2.49137) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67375 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-2.54446) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92040 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-2.79110) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69591 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.56661) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65548 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.52618) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66228 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-1.53298) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67070 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.54140) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86393 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-0.73463) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86330 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-0.73400) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65037 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-0.52107) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91018 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.78089) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53415 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-0.40485) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87258 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.74328) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38086 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.25156) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51893 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.38963) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46198 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.33268) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30230 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-1.17300) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44470 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-1.31540) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27520 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-1.14590) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84531 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.71601) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74398 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-0.61468) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80177 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-0.67247) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73696 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.60766) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50185 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.37255) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40958 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-0.28028) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63045 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.50115) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76901 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.63971) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47488 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.34558) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78441 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-0.65511) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59679 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-0.46749) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64082 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.51152) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54169 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.41239) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.41108 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-2.28178) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16498 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-2.03568) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.01635 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-2.88705) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45917 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-2.32987) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78210 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.65280) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67380 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.54450) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59535 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.46605) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37790 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.24860) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84504 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.71574) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70501 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.57571) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71282 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-0.58352) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43461 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.30531) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70068 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.57138) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47603 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-0.34673) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73304 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-0.60374) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54514 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-0.41584) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55314 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.42384) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75387 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.62457) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48492 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.35562) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22251 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-2.09321) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76650 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.63720) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39953 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-1.27023) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19346 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.06416) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43730 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.30800) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57295 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-1.44365) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41871 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-1.28941) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40434 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-1.27504) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46951 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-1.34022) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69210 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-1.56280) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16444 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-2.03514) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41830 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-1.28900) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64930 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.52000) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45427 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-2.32497) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36412 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-2.23482) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23726 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-2.10796) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74943 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-2.62013) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34432 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-0.21502) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51908 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.38978) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60953 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-0.48023) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53893 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.40963) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67219 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.54289) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59689 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-1.46759) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50701 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-1.37771) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78824 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-1.65894) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50454 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-1.37524) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38913 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.25983) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30236 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.17306) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58916 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.45986) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38225 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.25295) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46051 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-1.33121) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21786 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-1.08856) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37017 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-1.24087) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59463 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.46533) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59259 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-1.46329) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44127 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.31197) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46992 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.34062) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43253 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.30323) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05680 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-0.92750) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30470 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-1.17540) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54889 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.41959) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58772 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-1.45842) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21046 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-1.08116) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87062 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.74132) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29865 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-1.16935) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99778 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-0.86848) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15854 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.02924) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06807 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.93877) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28695 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.15765) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36968 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.24038) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55099 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-1.42169) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44192 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.31262) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47907 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-1.34977) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75333 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.62403) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71423 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.58493) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65733 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-1.52803) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72696 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-1.59766) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57311 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.44381) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89102 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.76172) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82588 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.69658) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53714 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-1.40784) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62437 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-1.49508) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08866 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-1.95936) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74821 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.61891) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33912 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-1.20982) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64840 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-1.51910) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83842 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-1.70912) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46592 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-1.33662) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96563 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-1.83633) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77850 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-1.64920) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42478 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.29548) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21354 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-1.08424) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34306 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.21376) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20377 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-1.07447) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17857 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-1.04927) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36377 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-1.23447) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41994 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.29064) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45229 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-1.32299) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44345 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.31415) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36959 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-1.24029) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34766 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-1.21836) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33743 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.20813) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38913 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-1.25983) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.58058 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-2.45128) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21386 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-2.08456) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37378 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-2.24448) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18349 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-2.05419) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28115 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-2.15185) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.46273 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-2.33343) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11323 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-1.98393) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17788 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-2.04858) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25073 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-2.12143) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51756 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-2.38826) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25154 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-2.12224) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.46409 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-2.33479) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.57971 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-2.45041) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16466 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-2.03536) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01932 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.89002) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31119 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-2.18189) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51125 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-2.38195) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17981 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-2.05051) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22303 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-2.09373) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28305 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-2.15375) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.39546 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-2.26616) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12925 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.99996) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26387 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-2.13457) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23753 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-2.10823) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89023 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-1.76093) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80217 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-1.67287) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64639 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-1.51709) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89184 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-1.76254) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83178 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-1.70248) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65096 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.52166) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76650 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.63720) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62546 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-1.49616) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45419 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.32490) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44146 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.31216) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53526 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-1.40596) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44358 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-1.31428) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56089 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-1.43159) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39389 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-1.26459) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35719 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-1.22789) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42981 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-1.30051) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51928 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-1.38998) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58037 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.45107) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59022 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-1.46092) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67099 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-1.54169) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42096 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-2.29166) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31122 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-2.18192) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06612 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-1.93682) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36839 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-2.23909) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21149 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-2.08219) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02095 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-1.89165) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.55604 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-2.42674) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18466 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-2.05536) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34175 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-2.21245) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66481 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.53551) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12428 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.99498) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06710 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-1.93780) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59232 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-1.46302) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21961 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.09031) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53825 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-1.40895) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28948 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-2.16018) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18098 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-2.05168) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.87196 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-2.74266) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.91294 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-2.78364) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.76499 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-2.63569) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.35352 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-3.22422) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28240 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-2.15310) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18509 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-2.05579) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85638 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.72708) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01823 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.88893) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93222 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.80292) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76194 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-0.63264) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62681 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-0.49751) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83742 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-0.70812) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86700 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-0.73770) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72504 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-0.59574) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35685 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-2.22755) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25032 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-2.12102) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10738 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-1.97808) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17543 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-2.04613) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68304 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-1.55374) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72653 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.59723) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23141 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-2.10211) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11391 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-1.98461) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55978 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.43048) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76169 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-0.63239) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63764 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-0.50834) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81802 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.68872) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24722 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-2.11792) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73093 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-1.60163) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63953 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-1.51023) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89397 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.76467) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85054 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.72124) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75932 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.63003) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77432 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.64502) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87429 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-0.74499) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76199 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.63269) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77543 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.64613) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69549 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.56619) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36061 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.23132) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42622 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.29692) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32777 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-1.19847) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43950 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-1.31020) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53976 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.41046) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61437 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.48507) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67464 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.54534) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68324 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.55394) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53314 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.40384) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60422 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-0.47492) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61903 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-2.48973) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91282 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-1.78352) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59848 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-0.46918) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38103 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.25173) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54365 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.41435) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09298 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-1.96368) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36002 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.23072) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59061 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.46131) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11764 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.98834) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85631 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-0.72701) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00687 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-0.87757) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29596 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-1.16666) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01405 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-0.88475) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99732 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.86802) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85182 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.72252) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87835 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.74905) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04730 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-0.91800) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90545 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-0.77615) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90186 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-0.77256) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96921 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-0.83991) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91726 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-0.78796) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94629 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.81699) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92861 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.79931) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98425 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-0.85495) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94847 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.81917) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95812 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-1.82882) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04748 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.91819) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02757 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-1.89827) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02857 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-1.89927) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17151 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-2.04221) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50475 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.37545) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54162 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.41233) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55118 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-1.42188) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58241 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.45312) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69428 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.56498) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72792 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.59862) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69951 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-0.57021) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67268 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.54338) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93352 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-1.80422) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98046 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.85116) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88585 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.75655) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78051 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.65121) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69678 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-1.56748) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23467 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-2.10537) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93772 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-0.80842) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96975 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.84045) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82520 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-0.69590) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75818 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-0.62888) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93549 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-0.80619) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92406 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.79476) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89212 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.76282) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94191 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.81261) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57274 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.44344) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55059 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.42129) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45905 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.32975) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42979 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.30050) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55880 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.42950) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66391 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.53461) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68473 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-1.55543) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32306 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-1.19376) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51591 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-1.38661) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88863 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.75933) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19678 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.06748) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09691 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-0.96761) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05881 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-0.92951) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90297 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.77367) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66625 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.53695) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50500 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-1.37570) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54878 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-1.41948) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53501 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.40571) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51828 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-1.38898) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56470 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-1.43540) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61365 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.48435) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00371 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.87441) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09277 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.96347) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04494 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.91564) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01881 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.88951) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96804 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.83874) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75413 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.62483) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75573 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-0.62643) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93059 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-0.80129) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00254 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-0.87324) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76986 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-0.64056) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17142 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-0.04212) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.22990 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.10060) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.66200 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.46730) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.95343 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.17587) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66067 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.53138) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51820 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.38890) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52113 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-1.39184) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40549 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.27619) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54119 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.41189) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46949 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.34019) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62916 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-1.49986) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81154 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.68224) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72852 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.59922) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79190 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.66260) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11936 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.99006) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94180 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.81250) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93726 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.80796) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86042 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-0.73112) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78681 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-0.65751) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84363 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-0.71433) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40960 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-1.28030) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56160 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-1.43230) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64568 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-1.51638) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83187 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-0.70257) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95468 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.82538) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79138 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.66208) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96238 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.83308) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69804 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.56875) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52965 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-1.40035) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58206 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.45276) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59227 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.46297) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50116 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.37186) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33253 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-1.20323) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44053 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-1.31124) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47044 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-1.34114) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47629 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.34699) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56002 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.43072) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48326 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.35396) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34170 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.21240) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50894 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.37964) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30189 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-1.17259) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14581 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-1.01651) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99609 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-0.86679) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25316 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.12386) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69657 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-1.56727) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54271 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-1.41341) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47009 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-1.34079) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64614 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-1.51684) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54182 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.41252) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65055 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-1.52125) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51169 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-1.38239) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16480 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-1.03550) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35686 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-1.22756) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21985 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-1.09055) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50693 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.37763) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35993 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-1.23063) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20377 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-1.07447) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46081 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-1.33151) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49964 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-1.37034) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48244 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-1.35314) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41926 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-1.28996) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17578 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-0.04648) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.03284 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (0.09646) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54090 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.41160) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37597 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-0.24667) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35230 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-0.22300) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37759 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.24830) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39131 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.26201) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38135 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.25205) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42034 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.29104) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40568 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.27638) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31000 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.18070) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42785 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.29855) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43942 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.31012) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49697 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.36767) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70176 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-1.57246) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30146 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-1.17216) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39501 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-1.26571) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41079 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-1.28149) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44682 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-1.31752) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71567 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-1.58637) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17397 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-1.04467) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07623 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.94693) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26265 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.13335) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23373 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.10443) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19008 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-1.06078) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31395 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.18465) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07457 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.94527) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13721 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.00791) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20984 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.08054) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40233 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.27303) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31419 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.18489) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50505 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.37575) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16913 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.03983) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31014 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-1.18084) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41705 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-1.28775) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41308 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-1.28378) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35150 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-1.22220) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40358 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-1.27428) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46353 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.33423) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41052 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.28122) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04785 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.91855) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28987 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-1.16057) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37294 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.24364) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27868 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.14938) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24322 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.11393) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57450 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.44520) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89508 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.76578) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04768 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.91838) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06945 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.94015) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00142 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.87212) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07585 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.94655) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46641 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-1.33711) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63384 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.50454) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76688 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.63758) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51069 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.38139) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56750 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-1.43820) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47645 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.34715) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55384 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.42454) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68938 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.56008) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26393 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-1.13463) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59692 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.46762) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61398 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-1.48468) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32519 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.19589) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68152 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.55222) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52679 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.39750) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52843 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.39913) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26649 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.13719) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31433 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-1.18503) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57085 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-1.44155) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35768 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.22838) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62617 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-1.49687) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19109 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.06179) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57259 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-1.44329) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14518 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.01588) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51333 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-1.38403) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45463 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.32533) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26712 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-1.13782) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52465 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.39535) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45509 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.32579) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44889 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-1.31959) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24214 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-1.11284) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14526 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-1.01596) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12129 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.99199) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20126 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-2.07196) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12381 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-1.99451) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00514 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.87584) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98446 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.85516) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26281 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-2.13351) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11225 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-1.98295) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24937 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-2.12007) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77728 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.64798) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32187 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-1.19257) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21822 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.08892) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06849 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.93919) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98708 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.85778) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96438 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-1.83508) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23859 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-2.10929) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09217 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.96287) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11459 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-1.98529) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23745 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-2.10815) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77312 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.64382) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83560 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-0.70630) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87720 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-0.74790) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82833 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.69903) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80863 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-0.67933) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17239 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-1.04309) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28635 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-1.15706) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43177 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-1.30247) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32861 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.19931) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26510 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-1.13580) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49801 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-1.36871) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56960 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-1.44030) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17506 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.04576) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21356 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-1.08426) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13715 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-1.00786) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46347 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-1.33417) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38794 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-1.25864) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44932 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-1.32002) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46198 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-1.33268) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42570 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-1.29640) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39670 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-1.26740) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28304 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-1.15374) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28728 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.15798) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35988 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-1.23058) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17185 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-1.04255) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40728 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-1.27798) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56459 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-1.43529) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30031 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-1.17101) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06583 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.93653) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17748 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.04818) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10981 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-0.98051) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29400 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-1.16470) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19933 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.07003) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21482 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-1.08552) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23478 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-2.10548) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10686 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.97756) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21658 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-2.08728) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37114 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-2.24184) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01023 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.88093) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97110 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.84180) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10517 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.97587) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93219 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.80289) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98327 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-1.85397) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94558 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-1.81628) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16498 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-2.03568) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81768 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-2.68838) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88328 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-2.75398) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.94571 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-2.81641) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.53078 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-3.40148) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75302 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-2.62372) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88364 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-2.75434) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80570 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-2.67640) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.48536 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-3.35606) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.79463 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-2.66533) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88078 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-2.75148) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.55728 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-3.42798) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.48299 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-3.35369) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20158 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-2.07228) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94183 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.81253) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01816 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.88886) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07190 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.94260) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10249 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-0.97319) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73186 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.60256) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86052 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.73122) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91856 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-1.78926) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68296 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.55366) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66560 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-1.53630) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70182 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-1.57252) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76321 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-1.63391) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.29538 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-2.16608) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80755 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-2.67825) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.68322 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-3.55392) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.93583 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-2.80653) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88606 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-2.75676) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11862 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-1.98932) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13500 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-2.00570) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.29663 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-2.16733) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21062 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-2.08132) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76335 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.63405) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99742 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.86812) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83280 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.70350) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92643 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.79713) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82468 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.69538) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92539 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-1.79609) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82302 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.69372) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83494 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.70564) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70220 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.57290) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36349 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-2.23419) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94824 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-1.81895) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95956 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-1.83027) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37759 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-2.24829) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37699 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-2.24769) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80529 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-2.67599) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.77661 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-2.64731) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81392 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-2.68462) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75631 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-2.62701) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34311 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-2.21381) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01840 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.88910) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17429 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-2.04499) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02316 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-1.89386) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09075 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-1.96145) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.52156 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-2.39226) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49840 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-2.36910) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49489 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-2.36559) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37840 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-2.24910) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07461 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-1.94531) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88117 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-1.75187) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87496 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.74566) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01914 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-0.88984) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74482 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.61552) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06845 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-0.93915) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83318 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.70388) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94910 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.81980) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19688 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-2.06758) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09298 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-1.96368) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79010 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-0.66080) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77500 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.64570) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79723 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-0.66793) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37799 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-2.24869) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68370 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.55440) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77251 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-1.64321) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64432 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.51502) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91099 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-1.78169) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66176 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-1.53246) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63578 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.50648) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87943 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.75013) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87788 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.74858) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72726 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-1.59796) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51947 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-1.39018) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68356 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-1.55426) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56432 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-1.43502) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60446 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-1.47516) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72827 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-1.59897) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51678 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.38748) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54524 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-1.41594) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44481 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.31551) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45297 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.32367) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59420 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.46490) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63433 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.50503) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66301 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-1.53372) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53920 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.40990) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22254 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-2.09324) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90745 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-2.77815) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.42884 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-3.29954) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88674 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-2.75744) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92624 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-0.79694) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01035 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-0.88105) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94510 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-0.81580) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79043 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.66113) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92627 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-0.79697) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73875 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.60945) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77739 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-0.64809) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63081 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-0.50151) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19013 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-2.06083) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16493 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-2.03563) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15674 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-2.02744) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79557 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.66627) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77864 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.64935) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89799 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.76869) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79505 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.66575) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87274 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.74344) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81537 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.68607) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93075 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.80145) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72519 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.59589) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10708 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-1.97778) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80173 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-2.67243) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19696 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.06766) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38289 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.25359) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.41326 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-2.28396) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81582 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.68652) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55211 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.42281) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71024 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.58094) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65687 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.52757) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70683 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-1.57753) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34044 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-2.21114) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77434 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.64504) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51716 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.38786) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84511 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-1.71581) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25560 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-2.12630) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71654 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-1.58724) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63165 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.50235) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69462 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.56532) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84863 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.71933) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93802 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.80872) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86354 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.73424) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01160 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.88230) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99734 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.86804) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74033 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.61103) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53078 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.40148) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80909 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.67979) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61176 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.48246) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88534 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.75604) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77810 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.64880) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73154 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.60224) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96256 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-1.83326) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.71944 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-2.59014) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19421 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-2.06491) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19902 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-2.06973) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49195 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.36265) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62033 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.49103) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72844 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-0.59914) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84488 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-0.71558) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70428 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-0.57498) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61686 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.48756) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23296 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-2.10366) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47784 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.34854) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73352 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-1.60422) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86457 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-1.73527) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88735 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.75805) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91984 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.79055) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90967 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.78037) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03944 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.91014) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10306 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.97376) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99868 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.86938) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94961 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-0.82031) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18826 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.05896) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81054 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-0.68124) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97672 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-0.84742) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00205 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.87275) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85587 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.72657) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09490 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-0.96560) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05149 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.92219) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86689 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.73759) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42391 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-1.29461) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64802 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.51872) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44013 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-1.31083) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50364 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-1.37434) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43858 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.30928) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74669 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-1.61739) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60786 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.47856) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49058 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-1.36128) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72830 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.59900) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83783 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.70853) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00659 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.87730) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91361 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.78431) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08480 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.95550) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12222 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.99292) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33555 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-1.20625) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46421 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-1.33491) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50160 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-1.37230) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39308 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-1.26378) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29621 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.16691) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71415 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-1.58485) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59346 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-1.46416) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51645 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-1.38715) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37849 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-1.24919) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51937 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-1.39007) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49071 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-1.36141) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25171 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-1.12242) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36679 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-1.23749) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57229 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-1.44299) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63556 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-1.50626) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46854 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-1.33924) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37980 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-1.25050) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39740 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-1.26811) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50266 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-1.37336) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63216 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-1.50286) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64889 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-1.51959) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58920 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.45990) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78308 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.65378) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90316 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.77386) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66199 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.53269) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95938 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.83008) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72765 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.59835) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98738 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.85808) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86292 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.73362) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46068 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.33138) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64901 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.51971) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89631 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.76701) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62547 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.49617) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85331 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.72401) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85315 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.72385) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60504 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.47574) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64623 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.51693) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82074 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.69144) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82096 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.69166) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95070 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.82140) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89399 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.76469) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76958 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.64028) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90423 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.77493) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72553 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.59623) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87944 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.75014) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02094 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.89164) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69636 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.56706) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70033 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.57103) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81005 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.68075) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78324 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-0.65394) | 1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75761 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.62831) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67829 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.54899) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71233 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.58303) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32285 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.19355) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44317 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.31387) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42927 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-1.29997) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37721 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.24791) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41721 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.28791) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26167 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-1.13237) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49497 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.36567) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71655 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.58725) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87903 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.74973) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81554 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.68624) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65916 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.52986) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33338 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.20409) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70928 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.57998) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80180 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.67250) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52642 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.39712) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39491 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.26561) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78289 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-0.65359) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64172 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.51242) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63870 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.50940) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46084 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.33154) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53404 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.40474) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93608 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.80678) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.64102 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-2.51172) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67357 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.54427) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10003 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.97073) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39058 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.26128) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70624 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.57694) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44220 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.31290) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54182 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.41252) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37788 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.24858) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39924 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.26994) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14221 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-2.01291) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33128 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-1.20198) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41134 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.28204) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69469 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.56539) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55548 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.42618) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95176 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.82246) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00760 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.87830) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97571 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.84641) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95892 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.82962) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16186 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-1.03256) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98115 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.85185) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06967 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.94037) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82101 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.69171) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89500 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.76570) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87108 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.74178) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89851 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.76921) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99846 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.86916) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85263 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.72333) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99228 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.86298) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70718 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.57788) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62478 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-1.49548) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56810 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-1.43880) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56462 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-1.43532) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48445 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-1.35515) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02087 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-1.89157) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69602 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-1.56672) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67126 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-1.54196) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60905 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-1.47976) | 1 | 1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78000 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-1.65070) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79355 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-1.66425) | -1 | -1 |
| G: -5278.76361 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60933 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-1.48003) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97954 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-1.85024) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80370 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-1.67440) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51044 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-1.38114) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59439 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-1.46509) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03919 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.90989) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19348 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-1.06418) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05568 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.92638) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05506 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-0.92576) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08113 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.95183) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02020 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.89090) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12222 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.99292) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22878 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.09948) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21484 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-1.08554) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14599 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-2.01669) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36918 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-2.23988) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07992 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-1.95062) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.33413 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-2.20483) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35187 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-2.22257) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06321 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-1.93391) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36330 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-2.23400) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47364 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-2.34434) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13402 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-2.00472) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19241 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-2.06311) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72144 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.59214) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62693 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-1.49763) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54326 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-1.41396) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75654 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-1.62724) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62639 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.49709) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55224 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.42294) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81785 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.68855) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73997 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.61067) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73170 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.60240) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12616 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.99686) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94053 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.81123) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59735 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-1.46805) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62631 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-1.49701) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64693 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.51763) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42388 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-1.29458) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18891 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.05961) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94697 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.81767) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02736 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.89806) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91778 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.78848) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02453 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.89523) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03996 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.91066) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00659 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.87730) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59929 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-1.46999) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53904 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-1.40974) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58998 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-1.46068) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97568 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.84638) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70585 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.57655) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07549 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.94619) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73541 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.60611) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13669 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.00739) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88806 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.75876) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97008 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-0.84078) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98140 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.85210) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20007 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.07077) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08831 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.95901) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97612 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.84682) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90213 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.77283) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00210 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.87281) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83214 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.70284) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87652 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-0.74722) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94112 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.81182) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60640 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-0.47710) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80172 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.67242) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87086 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.74156) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76939 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-0.64009) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80251 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.67321) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80422 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.67492) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60142 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.47212) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54734 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.41804) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48674 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.35744) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49074 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.36144) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08793 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-0.95863) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91236 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.78306) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90270 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.77340) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07928 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-0.94998) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53569 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.40639) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46157 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-1.33227) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70985 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.58055) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65948 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.53018) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66100 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-1.53170) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66130 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.53200) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64938 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.52008) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90096 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-0.77166) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83982 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.71052) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91935 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-0.79006) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70092 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-1.57162) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54894 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.41965) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57518 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.44588) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61188 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.48259) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00338 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.87408) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88559 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-0.75629) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86474 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-0.73544) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88833 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.75903) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97959 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.85029) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04816 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.91887) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97965 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.85035) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22534 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-2.09604) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14153 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-2.01223) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59096 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-1.46166) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51022 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.38092) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81945 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.69015) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73031 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-1.60101) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81564 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.68634) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79132 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.66202) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44505 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-1.31575) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56595 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.43665) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32102 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-1.19172) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47120 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.34190) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07781 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.94851) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47896 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-1.34966) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30946 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-1.18016) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26355 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-1.13425) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15804 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-2.02874) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31138 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-2.18208) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08310 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.95380) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08068 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.95138) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12906 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.99976) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03755 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.90825) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24779 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-2.11849) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05051 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.92121) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23249 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-2.10320) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30134 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-2.17204) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04542 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.91612) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07089 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.94159) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.41419 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-2.28489) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06833 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-1.93903) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13309 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-2.00379) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99312 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.86382) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26243 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-2.13313) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73997 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-1.61067) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63262 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-1.50332) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96754 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-1.83824) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47825 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.34895) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82449 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.69519) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49787 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.36857) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33449 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.20519) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45999 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.33069) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72933 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.60003) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69787 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-1.56857) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75156 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-1.62226) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69417 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.56487) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54576 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.41646) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75224 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.62294) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66511 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.53581) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56911 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.43981) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36736 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-1.23806) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82968 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.70039) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48679 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.35749) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15618 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.02688) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64353 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-1.51423) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37983 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-1.25053) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46353 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-1.33423) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64729 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-1.51799) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56965 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-1.44035) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60315 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.47385) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67292 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.54362) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99810 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.86880) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44795 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-2.31865) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22566 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-2.09637) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38270 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-2.25340) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.33427 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-2.20497) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21630 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-2.08700) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19922 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-2.06992) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26096 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-2.13166) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.29315 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-2.16385) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06427 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.93497) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03293 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.90363) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38689 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-2.25759) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.27767 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-2.14837) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21366 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-2.08436) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40537 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-2.27607) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12629 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-1.99699) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12082 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.99152) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22020 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-2.09090) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92593 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-1.79663) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99176 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-1.86246) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95641 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-1.82711) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90356 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.77426) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09086 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.96156) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93374 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.80444) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08923 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-1.95993) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08855 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-1.95925) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98577 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-1.85647) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18964 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-2.06034) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14879 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-2.01949) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26893 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-2.13963) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07785 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-1.94855) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15500 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-2.02570) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13301 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-2.00371) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64144 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.51214) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74854 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-1.61924) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73485 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-1.60555) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65180 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-1.52250) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74340 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-1.61410) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63953 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-1.51023) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90196 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-1.77266) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74699 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.61769) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64878 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.51948) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55425 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.42495) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35000 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.22070) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47626 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.34696) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46296 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.33366) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51145 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.38215) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58443 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-1.45513) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62108 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.49178) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63548 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-1.50618) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65287 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.52357) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58636 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-1.45706) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63537 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.50607) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74615 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.61685) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84356 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.71426) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83970 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.71040) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64013 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.51083) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77426 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.64496) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50349 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-2.37419) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19508 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-2.06578) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30896 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-2.17966) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28967 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-2.16037) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.54115 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-2.41185) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20784 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-2.07854) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09921 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-1.96991) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53052 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.40122) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26181 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-1.13251) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44913 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.31983) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59616 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-1.46686) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42524 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-1.29594) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41667 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-1.28737) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28997 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.16067) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42970 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.30040) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43792 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-1.30862) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53909 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-1.40979) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15317 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-2.02387) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18961 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-2.06031) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32270 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-2.19340) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16403 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-2.03473) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13083 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-2.00153) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13244 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-2.00314) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14781 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-2.01851) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85622 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.72692) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18376 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-2.05446) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69125 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-2.56195) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.87931 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-2.75001) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.79819 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-2.66889) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.99509 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-2.86579) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.29058 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-3.16128) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81544 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-2.68614) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.91651 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-2.78721) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.40430 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-3.27500) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69495 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-2.56565) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88271 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-2.75341) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59109 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-2.46179) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86717 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-2.73787) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.29496 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-3.16566) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.18323 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-3.05393) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.84380 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-2.71450) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.95303 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-2.82373) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.83789 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-2.70859) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.71471 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-2.58541) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98465 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.85535) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12087 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-1.99157) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08923 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-1.95993) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47775 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-2.34845) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40521 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-2.27591) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59321 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-2.46391) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51577 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-2.38647) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49574 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-2.36644) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.33715 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-2.20785) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13342 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-2.00412) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.73093 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-2.60163) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.35208 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-3.22278) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80973 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-2.68043) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.91302 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-2.78372) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.60619 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-2.47689) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19551 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-2.06621) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12866 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-1.99936) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06493 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.93563) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49186 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-1.36256) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42481 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.29551) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42347 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-1.29417) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62753 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-1.49823) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30708 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-2.17778) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.29206 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-2.16276) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75706 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-1.62776) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56002 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.43072) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52546 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-1.39616) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53014 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.40084) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75328 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-1.62398) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63072 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-1.50142) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78835 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-1.65905) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74404 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-2.61474) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.73313 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-2.60383) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.73011 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-2.60081) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59696 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-2.46766) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33231 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.20302) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49839 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-1.36909) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34510 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-1.21580) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54100 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-1.41170) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57360 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-1.44430) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43365 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-1.30435) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39316 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-1.26386) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42572 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-2.29642) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.43383 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-2.30453) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11932 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-1.99002) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21707 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-2.08777) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44695 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-2.31765) | -1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42303 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-2.29373) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.57732 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-2.44802) | 1 | -1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36697 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-2.23767) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.06451 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-2.93521) | 1 | 1 |
| G: -5278.76361 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51215 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-2.38285) | 1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38455 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-2.25525) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35944 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-2.23014) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17217 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-2.04287) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16730 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-2.03800) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12468 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-1.99538) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98188 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-1.85258) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79377 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-0.66447) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76441 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.63511) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93410 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-0.80480) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75220 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.62290) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65764 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-0.52834) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87263 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.74333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98902 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.85972) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72002 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-1.59072) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38814 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-2.25884) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95086 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-1.82156) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77159 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-1.64229) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64769 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.51840) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79097 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-0.66167) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18385 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-1.05455) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79372 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.66442) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75467 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.62537) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87037 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.74107) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13405 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.00475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96978 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.84048) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02755 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.89825) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92148 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.79218) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88161 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.75231) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82727 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.69797) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00662 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-0.87732) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57651 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.44721) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44824 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-1.31894) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56285 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.43355) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36010 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-1.23080) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68334 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-1.55404) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44579 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-1.31649) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62397 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-1.49467) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73639 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.60709) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91369 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.78440) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78918 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-0.65988) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75633 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.62703) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76186 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.63256) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69821 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.56891) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84841 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.71912) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72283 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.59353) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57519 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.44589) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68955 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.56026) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54933 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.42003) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85119 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.72189) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63083 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.50153) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70449 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.57519) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04678 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-1.91748) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78363 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-2.65433) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97505 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-1.84575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00503 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-1.87574) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69282 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.56352) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61051 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.48121) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51986 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.39057) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65614 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.52684) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62602 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.49672) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64632 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.51702) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14906 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-2.01977) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49683 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-1.36754) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67262 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-1.54332) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60271 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-1.47341) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66288 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-1.53358) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60554 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.47624) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83235 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.70305) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72125 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-1.59195) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03230 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-1.90300) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72280 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-1.59350) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56745 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-1.43815) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71072 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.58142) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92302 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-1.79372) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69401 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-1.56471) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41493 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.28563) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78364 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.65434) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56383 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.43453) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54527 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-1.41597) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65278 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-1.52348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40856 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-1.27926) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90999 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.78069) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55738 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-1.42808) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74982 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-1.62052) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53950 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.41020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31400 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-1.18470) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64916 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.51986) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64288 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-1.51358) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75638 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.62708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63812 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.50882) | 1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72835 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.59905) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72734 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.59804) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69972 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-1.57042) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63657 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.50727) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69393 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-1.56463) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66731 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.53801) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70775 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-1.57845) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52492 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-1.39562) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38380 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-1.25450) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47825 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-1.34895) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41501 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-1.28571) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42723 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-1.29793) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43155 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-1.30226) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62965 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-1.50035) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56998 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-1.44068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38725 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.25796) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60500 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.47570) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51120 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-1.38190) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73240 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.60310) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55757 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.42827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35544 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-1.22615) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51781 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-1.38852) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42832 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.29902) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77964 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.65034) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60032 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-1.47102) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38761 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.25831) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60704 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.47774) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27863 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.14933) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49950 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.37020) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36423 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.23493) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57591 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.44661) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52266 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.39336) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16379 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.03450) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50312 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.37382) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57760 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.44830) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21925 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.08995) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33319 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.20389) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69240 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.56310) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41858 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.28928) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55270 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.42340) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51735 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.38805) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74674 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.61744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90152 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.77222) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43577 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.30647) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74176 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-1.61247) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57226 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.44297) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31797 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.18867) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31444 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-1.18514) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73439 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-1.60509) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61545 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.48615) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36181 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.23251) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80870 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-1.67941) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75028 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-1.62098) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24088 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-1.11159) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50143 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-1.37213) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48717 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-1.35788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64405 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-1.51475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42399 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-1.29469) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11822 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-0.98892) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06017 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.93087) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54339 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.41409) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36132 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.23202) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52424 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.39494) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54571 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.41641) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67243 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.54313) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84914 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-1.71984) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72781 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.59851) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60492 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.47562) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68163 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.55233) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66916 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.53987) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72881 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.59951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58671 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.45741) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73877 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.60947) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34033 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-2.21103) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.33220 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-2.20290) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24738 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-2.11808) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30531 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-2.17601) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96925 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.83995) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07173 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-1.94243) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16150 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-2.03220) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00778 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-1.87848) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24011 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-2.11081) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.39010 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-2.26080) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15717 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-2.02787) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09859 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.96929) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42807 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-1.29877) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43664 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-1.30734) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53991 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-1.41061) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46187 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-1.33257) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37487 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-1.24557) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58993 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.46063) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44682 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.31752) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55343 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.42414) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44804 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.31875) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32082 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-2.19152) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22332 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-2.09403) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00528 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.87598) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32885 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-2.19955) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12022 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.99092) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89959 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.77029) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17666 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-2.04736) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13184 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-2.00254) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08757 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.95827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22186 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-2.09256) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15331 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-2.02401) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30953 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-2.18023) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12849 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-1.99919) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90030 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-1.77100) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65662 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.52732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88813 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.75884) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80201 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.67271) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16074 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-2.03144) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96501 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-1.83571) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79959 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-1.67029) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95839 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-1.82909) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.87991 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-2.75061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.79471 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-2.66541) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.15559 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-3.02629) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.41982 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-2.29052) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67223 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-2.54293) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.58725 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-2.45795) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47974 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-2.35044) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.43334 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-2.30404) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.89749 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-2.76819) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.14985 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-3.02055) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.53802 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-2.40872) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96729 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-1.83799) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79537 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-1.66607) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.01294 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-2.88364) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69223 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-2.56293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.70429 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-2.57499) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61463 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-1.48533) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65365 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.52435) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66887 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-1.53957) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77123 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-1.64194) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45729 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-2.32799) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42129 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-2.29199) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.31236 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-2.18306) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36654 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-2.23724) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.52638 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-2.39708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.42643 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-2.29713) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51220 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-2.38290) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40197 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-2.27267) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20109 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-2.07179) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35870 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-2.22940) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37653 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.24723) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37732 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-1.24802) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17680 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.04750) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54636 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.41706) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28274 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-1.15344) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62446 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.49516) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60282 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-1.47352) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36399 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.23469) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57033 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.44103) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35267 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.22337) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78274 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-2.65344) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.53081 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-2.40151) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51038 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-2.38108) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61343 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-2.48413) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31085 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.18155) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13060 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.00130) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26554 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.13624) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43126 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.30196) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38383 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-1.25453) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35147 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.22217) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26097 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.13167) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.04617 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-2.91687) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28632 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-2.15702) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14874 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-2.01944) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.27579 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-2.14649) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40238 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.27308) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41757 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-1.28827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48688 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-1.35758) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91480 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.78550) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65194 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.52264) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36072 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.23142) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74201 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.61271) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56791 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.43861) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63673 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-1.50743) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60350 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.47420) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61452 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.48522) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61458 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.48528) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39155 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-1.26225) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45474 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.32544) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70304 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-1.57374) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72040 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.59110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54402 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.41472) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43547 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.30617) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38432 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.25502) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41041 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.28111) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93137 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.80207) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41683 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.28753) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40513 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.27583) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62350 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.49420) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55692 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.42762) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71564 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.58634) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52701 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.39771) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68342 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.55412) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41030 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.28100) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38584 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.25654) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40290 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.27360) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60405 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.47475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25495 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.12565) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26238 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-1.13308) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41672 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.28743) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39449 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-1.26519) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18793 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-1.05863) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20897 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.07967) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24227 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.11297) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50905 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-1.37975) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51069 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-1.38139) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32720 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.19790) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25612 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.12682) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41996 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.29066) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33196 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-1.20266) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24124 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-1.11194) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42375 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-1.29445) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41343 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.28413) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60946 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.48016) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57246 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-1.44316) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49371 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-1.36441) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48524 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-1.35594) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31795 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-1.18865) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80114 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.67184) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52538 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.39608) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54660 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-1.41731) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74079 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-1.61149) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87374 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.74444) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14671 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.01741) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59161 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.46231) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33101 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-1.20171) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.52026 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-2.39096) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.02628 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-2.89698) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.14100 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-3.01170) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.46654 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-2.33724) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45152 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-2.32222) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63375 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-2.50445) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66144 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.53214) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75357 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.62427) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79303 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.66373) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41482 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.28552) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46639 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.33709) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46288 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.33358) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52347 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-1.39418) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31697 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-1.18767) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43702 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-1.30772) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66565 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.53635) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55425 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-1.42495) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46418 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-1.33488) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48366 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-1.35437) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22063 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-2.09133) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.26490 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-2.13560) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21541 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-2.08611) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.36703 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-2.23773) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50219 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-2.37289) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30206 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.17276) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39757 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-1.26827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22448 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-1.09518) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42217 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-1.29287) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00197 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.87267) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45074 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-1.32144) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36377 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-1.23447) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33811 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-1.20881) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24086 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-1.11156) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31392 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-1.18462) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76002 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-1.63072) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62424 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-1.49494) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69404 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-1.56474) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56127 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-1.43197) | 1 | 1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37144 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-1.24215) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48269 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-1.35339) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88690 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-2.75760) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.21535 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-2.08605) | 1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40823 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-2.27893) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.39914 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-2.26984) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51549 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-2.38619) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80508 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-2.67578) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14189 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-1.01259) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19283 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-1.06353) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57738 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-1.44808) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34282 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-1.21352) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51637 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-1.38707) | 1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45172 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-1.32242) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86115 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.73185) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19471 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.06541) | -1 | -1 |
| G: -5278.76361 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96657 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.83727) | 1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48060 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.35130) | 1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88893 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-0.75963) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84058 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.71128) | 1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23000 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.10070) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01669 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.88739) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68648 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.55718) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85810 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.72880) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63780 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.50850) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97927 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.84997) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77560 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.64630) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17604 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.04674) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94964 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.82034) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68708 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.55778) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71671 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.58741) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03756 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-0.90826) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.08209 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-2.95279) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.87740 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-2.74811) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.20835 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-3.07905) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91380 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-1.78450) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88381 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.75451) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03750 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-1.90820) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48140 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-2.35210) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86889 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-2.73959) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12757 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-1.99827) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19141 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-2.06211) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17102 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-2.04172) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15421 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-2.02491) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.66390 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-2.53460) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96452 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.83522) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09535 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.96605) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82724 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.69794) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12800 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.99870) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.56545 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-2.43615) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02879 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.89949) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78919 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.65989) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02389 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-1.89459) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00566 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.87636) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.60896 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-2.47966) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80756 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-1.67826) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20400 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-2.07470) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61408 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-2.48478) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05657 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.92727) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13312 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.00382) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16547 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-2.03617) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.65618 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-2.52688) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19791 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-2.06861) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22732 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-2.09803) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16634 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-2.03704) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72238 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-2.59308) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00291 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.87361) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17736 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-2.04806) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99728 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-1.86798) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84732 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.71802) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.58088 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-2.45158) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.57171 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-2.44241) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59452 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-2.46522) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.27967 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-3.15037) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72810 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-2.59880) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.26626 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-3.13696) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.00065 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-2.87135) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96550 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-1.83620) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05483 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-1.92553) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13644 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-2.00714) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67822 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-2.54892) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.52733 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-2.39803) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93861 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-1.80931) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95361 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.82431) | 1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05372 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.92442) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63130 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-2.50201) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49234 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-2.36304) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96476 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.83546) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86103 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.73173) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.76276 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-2.63346) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.54107 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-2.41177) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71768 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-1.58838) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.33529 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-3.20599) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95298 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-1.82368) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59110 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.46180) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62186 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-2.49256) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49087 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-2.36157) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94073 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-1.81143) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92546 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-2.79616) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85617 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.72687) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57984 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.45054) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19697 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.06767) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84752 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.71822) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.13183 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-3.00253) | 1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80031 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.67101) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80743 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.67813) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86643 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.73713) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47244 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.34314) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50755 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-2.37825) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77258 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.64328) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63159 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.50229) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79211 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.66281) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47581 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.34651) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19098 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.06168) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43962 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.31032) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86602 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.73672) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72407 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-2.59477) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43637 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.30707) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41136 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.28206) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67123 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.54193) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33800 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.20870) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09707 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.96777) | -1 | -1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23014 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.10084) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87603 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.74673) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64833 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.51903) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77437 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.64507) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47633 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.34703) | 1 | 1 |
| G: -5278.76361 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.43993 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-2.31063) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07819 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.94889) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02431 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.89501) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03460 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.90530) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68634 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.55704) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.02263 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-2.89333) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95127 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.82197) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75951 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-1.63021) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17511 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-2.04581) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76604 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-1.63674) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78333 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-2.65404) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64172 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.51242) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64996 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.52066) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79802 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.66872) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56980 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.44050) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17043 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.04113) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00913 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.87983) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16616 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.03686) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90472 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.77542) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75024 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.62094) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66177 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.53247) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84275 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.71346) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62370 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.49440) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.37911 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-2.24981) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60044 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.47114) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77511 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.64581) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70229 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.57299) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41788 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.28858) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37401 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.24471) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40999 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.28069) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21238 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.08308) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58968 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.46038) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61480 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.48550) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91015 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.78085) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59624 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.46694) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.83683 HOMO: -6.52801 LUMO: -0.28028 factor:1 | -1 (0.29247) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.96796 HOMO: -7.22462 LUMO: 0.52518 factor:1 | -1 (0.16134) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.62698 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.50232) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14280 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.01350) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45831 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.32901) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31036 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.18106) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68855 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.55925) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54468 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.41538) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43178 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.30248) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77622 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.64692) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.25374 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.12444) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.16742 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.03812) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50591 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.37661) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70273 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.57343) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68780 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.55850) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80936 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.68006) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51360 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.38430) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96376 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.83446) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.53098 HOMO: -6.23957 LUMO: 1.78507 factor:1 | -1 (0.59832) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.64515 HOMO: -6.35114 LUMO: 1.92112 factor:1 | -1 (0.48414) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.37070 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.75860) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.96102 HOMO: -6.60420 LUMO: 1.78779 factor:1 | -1 (0.16828) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.25469 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.12539) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37583 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.24654) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08764 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.04166) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59774 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.46844) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95031 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.82101) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.85153 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.72223) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10702 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.97772) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85317 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.72387) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64119 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.51189) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58696 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.45766) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73684 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.60754) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48481 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.35551) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49913 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.36983) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34857 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.21927) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61717 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.48787) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47075 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.34145) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36506 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.23576) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.13975 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.01045) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60289 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.47359) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86549 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.73620) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97603 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.84673) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75084 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-2.62154) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89842 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.76912) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15285 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-2.02355) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84424 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.71494) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68955 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.56025) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83768 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.70839) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51058 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.38128) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90141 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.77211) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63833 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.50903) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80422 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.67492) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61521 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.48591) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61304 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.48374) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81489 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.68559) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54406 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.41476) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16524 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.03594) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87984 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.75054) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33706 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.20776) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66153 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.53223) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43227 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.30297) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.19950 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.07021) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79241 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.66311) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80887 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.67957) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82824 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.69894) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60397 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.47467) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39730 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.26800) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.27382 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.14452) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47124 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.34194) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.88377 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-2.75447) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.45538 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-2.32608) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47381 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.34451) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61091 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.48161) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63327 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.50397) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33114 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.20185) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48799 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.35869) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64519 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.51589) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67393 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.54463) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28382 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.15452) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57744 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.44814) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44679 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.31749) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34510 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.21580) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51120 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.38190) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71015 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.58085) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57791 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.44861) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86554 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-2.73624) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59676 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.46746) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81954 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.69024) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55785 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.42855) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35900 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.22970) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68542 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.55612) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32223 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.19293) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61144 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.48214) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42345 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.29416) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59527 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.46597) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43837 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.30907) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44759 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.31829) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02880 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.89950) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84338 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.71408) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45203 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.32273) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51469 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.38539) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56670 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.43740) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51147 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.38218) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41898 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.28968) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28140 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.15210) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47858 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.34928) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81920 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-2.68990) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50927 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.37997) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24273 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-2.11343) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27985 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.15055) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55923 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.42993) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40975 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-2.28045) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51340 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.38410) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70797 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.57867) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72424 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.59494) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79681 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.66751) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55569 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.42639) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10340 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.97410) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.95896 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-2.82966) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08629 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.95699) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16175 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-2.03245) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83379 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.70449) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61513 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.48583) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77674 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.64744) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52849 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.39919) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71255 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.58325) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48248 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.35318) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68185 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.55255) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33208 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.20278) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.87618 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.25312) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.07480 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.05450) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26476 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.13546) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26783 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.13853) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39437 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.26507) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.87063 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.25867) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10984 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.01946) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.72344 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (0.40586) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.01621 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (0.11309) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.64290 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (0.48640) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.64554 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (0.48376) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28653 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.15723) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.78371 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.34558) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.81289 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (0.31641) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.20787 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (0.92143) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77636 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.64706) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00230 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.87300) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16741 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.03811) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22554 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.09624) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70286 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.57356) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98219 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.85289) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26774 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.13844) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69116 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.56186) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85663 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.72733) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58923 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.45993) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74387 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.61457) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81304 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.68374) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75766 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.62837) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63497 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.50567) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48147 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.35217) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66297 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.53367) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53404 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.40474) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38139 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.25209) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81350 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.68420) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45184 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.32254) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85037 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.72107) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66370 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.53440) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52895 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.39965) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58109 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.45179) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33412 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.20482) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.29191 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.16262) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20350 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.07420) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32312 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.19382) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20148 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.07218) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31618 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.18688) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40843 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.27913) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08518 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.95588) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10695 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.97765) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42331 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.29401) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78206 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.65277) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97219 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.84289) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92449 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.79519) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77020 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.64090) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04808 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.91878) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07029 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.94099) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.06571 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-2.93641) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19843 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-2.06913) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91181 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.78251) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17843 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-2.04913) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05249 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.92319) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24319 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-2.11389) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17532 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-2.04602) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88163 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.75233) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85431 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.72501) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06280 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.93351) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04816 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.91887) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97431 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.84501) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71254 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.58324) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00359 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.87429) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68568 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.55638) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86794 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.73864) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88748 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.75818) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53768 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.40838) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74342 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.61412) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82996 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-1.70066) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83809 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.70879) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88862 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.75932) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61463 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.48533) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70496 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.57566) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52038 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.39108) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05606 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.92677) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87310 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.74380) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66662 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.53732) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64735 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.51805) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50370 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.37440) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36239 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.23309) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77854 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.64924) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05695 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.92765) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10942 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.98012) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.19141 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-2.06211) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85913 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.72983) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60283 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.47353) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86069 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.73139) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78782 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.65852) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73151 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.60222) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44555 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.31625) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73244 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.60314) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58356 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.45426) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20115 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-2.07185) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81238 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.68308) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68214 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.55284) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44848 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.31918) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69821 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.56891) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84474 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.71544) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84822 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.71892) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89135 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.76205) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98044 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.85114) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83693 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.70763) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63203 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.50273) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60974 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.48044) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96447 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.83517) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79674 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.66744) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94300 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.81370) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65453 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.52523) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91650 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.78720) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60463 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.47533) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65070 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.52140) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53875 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.40945) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61007 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.48077) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75396 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.62466) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62441 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.49511) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70292 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.57362) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91160 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.78230) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71957 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.59027) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80142 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.67212) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66479 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.53549) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95642 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.82712) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99495 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.86565) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63832 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.50902) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61559 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.48629) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95974 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.83044) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04951 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.92021) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18567 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.05637) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77220 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.64290) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11827 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.98897) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25354 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.12424) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46747 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.33817) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50788 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.37858) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48919 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.35989) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65281 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.52351) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49556 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.36626) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24464 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.11534) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53558 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.40628) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61636 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.48706) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57910 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.44980) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89250 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.76320) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81835 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.68905) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78207 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.65277) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74180 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.61250) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40046 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.27116) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48642 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.35712) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74863 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.61933) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17870 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-2.04940) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82190 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.69260) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95350 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.82420) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96087 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.83157) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70595 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.57665) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.68303 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-2.55373) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69381 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-2.56451) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.57807 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-3.44877) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.33630 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-3.20700) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.89887 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.76957) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.53724 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-2.40794) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10825 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.97895) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18232 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-2.05302) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06060 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.93130) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78139 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.65209) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65706 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.52776) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81622 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.68692) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85285 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.72355) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83851 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.70921) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80099 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.67169) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66368 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.53438) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49222 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.36292) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90755 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.77825) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61659 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.48729) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50195 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.37265) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72459 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.59529) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85257 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.72327) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52154 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-1.39224) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52954 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.40024) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20616 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-1.07686) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57420 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.44490) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53284 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.40354) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69096 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.56166) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30987 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-1.18057) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31109 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-1.18179) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98755 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.85825) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49305 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-1.36375) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61776 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-1.48846) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14343 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-2.01413) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07625 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-1.94695) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06321 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-1.93391) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88922 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-1.75992) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81491 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-1.68561) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07739 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-1.94809) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81248 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-2.68318) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.34296 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-3.21366) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50888 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-2.37958) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72284 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-2.59354) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.87155 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-2.74225) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50975 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-2.38045) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66761 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-1.53831) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92482 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-1.79552) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88588 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-1.75658) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47953 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-1.35023) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77162 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-1.64232) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06980 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-1.94050) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84272 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-1.71342) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77042 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-1.64112) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53232 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.40302) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98882 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-1.85952) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00223 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-1.87293) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.66118 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-2.53188) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67733 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-1.54803) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80302 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.67372) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92560 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-1.79631) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76552 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-1.63622) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57550 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-1.44620) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.50455 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.62475) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.34675 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (0.78255) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.70570 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (0.42360) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.60026 HOMO: -6.86815 LUMO: 2.47896 factor:1 | -1 (0.52904) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21355 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.08425) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.06358 HOMO: -6.58788 LUMO: 2.30208 factor:1 | -1 (0.06572) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39028 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.26098) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51818 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.38888) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85232 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-1.72302) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.99183 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-2.86253) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97701 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-1.84771) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64786 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-1.51856) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52263 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-1.39333) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66780 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-1.53850) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35434 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.22504) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49872 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.36942) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54898 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.41968) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50512 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.37582) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55769 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.42839) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51003 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.38073) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80773 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-1.67843) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75792 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-2.62862) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03970 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-1.91040) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77412 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-1.64482) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05393 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.92463) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85213 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-1.72283) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88800 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.75870) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57983 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-1.45053) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80778 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-1.67848) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73526 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-1.60596) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85352 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.72422) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94955 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.82025) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52111 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-1.39181) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43052 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-1.30122) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70361 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-1.57431) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60214 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.47284) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26331 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-1.13401) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80020 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.67090) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71002 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.58072) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70950 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.58020) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78493 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.65563) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43260 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.30330) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38348 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.25418) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55004 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.42074) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66343 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.53413) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63581 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.50651) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74711 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.61781) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80006 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.67076) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.29643 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.16713) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49401 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.36471) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45652 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.32722) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72607 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.59677) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54076 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.41146) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33317 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.20387) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.18394 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.05464) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61048 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.48118) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40019 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.27089) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77788 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.64858) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03143 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.90213) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01712 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-1.88782) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18300 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-2.05370) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86928 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-1.73998) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58240 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.45310) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88052 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.75122) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64534 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.51604) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80629 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.67699) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42609 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.29679) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.19989 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.07059) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63647 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.50717) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62765 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-0.49835) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34343 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.21413) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43366 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.30436) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69954 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.57024) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62041 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.49111) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58652 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.45722) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23737 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-2.10807) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59390 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.46460) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78868 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.65938) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43675 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.30745) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69080 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-1.56150) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37955 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-1.25025) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30237 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-2.17307) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45009 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-1.32079) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59139 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-1.46209) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92522 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-1.79592) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05216 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-1.92287) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73570 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-1.60640) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78582 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-1.65652) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61260 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-0.48330) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39801 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.26871) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39311 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-0.26381) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.29842 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.16912) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55872 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.42942) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82352 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.69422) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38969 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.26039) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63376 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.50446) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75363 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-1.62433) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62995 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-1.50065) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72462 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-1.59532) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51855 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-1.38925) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43534 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-1.30604) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64685 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.51755) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15911 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-2.02981) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37000 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.24070) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57020 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.44090) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.40387 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-2.27457) | 1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18460 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-2.05530) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14109 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-2.01179) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44820 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-2.31890) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77086 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.64156) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52465 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.39535) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71568 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.58638) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98325 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.85395) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64697 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.51767) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53393 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.40463) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26849 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.13919) | -1 | -1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49956 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.37027) | 1 | 1 |
| G: -5278.76361 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34427 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.21497) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17605 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.04675) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30745 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.17815) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49393 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.36463) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55889 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.42959) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31570 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.18640) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.18960 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.06030) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19710 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.06780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26249 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.13319) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47327 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.34397) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31534 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.18604) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04026 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.91096) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22946 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.10016) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37221 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.24291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57870 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.44940) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72817 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.59887) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68945 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.56015) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93473 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.80543) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77557 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.64627) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47241 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.34311) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50231 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.37301) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30589 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.17659) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24151 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.11221) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40081 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.27151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10768 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.97839) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22439 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.09510) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.87923 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.25007) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17613 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.04683) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.19099 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.06169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10361 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.02569) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25090 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.12160) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08420 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.95490) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31582 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.18653) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06766 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.93836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92501 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.79572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32905 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.19975) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29016 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.16086) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37223 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.24293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06107 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.93177) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06616 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.93686) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32380 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.19450) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19212 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.06282) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17544 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.04614) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56783 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.43853) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17687 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.04757) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.93988 HOMO: -6.60420 LUMO: 1.78779 factor:1 | -1 (0.18942) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35915 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.22985) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.12954 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.00024) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08179 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.04751) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14122 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.01192) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.91414 HOMO: -6.82734 LUMO: -0.60137 factor:1 | -1 (0.21516) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.04130 HOMO: -7.18653 LUMO: 0.59321 factor:1 | -1 (0.08800) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08707 HOMO: -7.29265 LUMO: 0.48164 factor:1 | -1 (0.04223) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89848 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.76918) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06834 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.93904) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24369 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.11439) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25046 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.12116) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24581 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.11651) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36532 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.23602) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16230 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.03300) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85021 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.72091) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30361 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.17431) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84569 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.71639) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78079 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.65150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03247 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.90317) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78414 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.65484) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09296 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.96366) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84904 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.71974) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93914 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.80984) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65750 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.52820) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59880 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.46951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83914 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.70984) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04289 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.91360) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85968 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.73038) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80387 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.67457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92667 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.79738) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09022 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.96092) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69078 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.56148) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57396 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.44466) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51943 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.39013) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45523 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.32593) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44097 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.31167) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46165 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.33235) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90675 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.77745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47351 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.34422) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50954 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.38024) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51003 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.38073) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72400 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.59470) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24733 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.11803) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23778 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.10848) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39610 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.26680) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57637 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.44707) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59657 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.46727) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53989 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.41059) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34620 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.21690) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93593 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.80663) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21733 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.08803) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54531 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.41601) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68153 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.55223) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84129 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.71199) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76115 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.63185) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81484 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.68554) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93930 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.81000) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66545 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.53615) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80090 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.67160) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78713 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.65784) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75584 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.62654) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02039 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.89109) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01868 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.88938) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98934 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.86004) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57766 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.44836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54893 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.41963) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75700 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.62770) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40516 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.27586) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51066 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.38136) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42353 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.29423) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82223 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.69293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68666 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.55736) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27501 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.14571) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30804 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.17874) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53931 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.41001) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40739 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.27809) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53232 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.40302) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65096 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.52166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93080 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.80150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57001 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.44071) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33966 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.21036) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15452 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.02522) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57327 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.44397) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84545 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.71615) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68300 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.55370) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83092 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.70162) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99617 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.86687) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54199 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.41269) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43820 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.30890) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74481 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.61551) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27068 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.14138) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51379 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.38449) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36380 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.23450) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83238 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.70308) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63477 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.50547) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34374 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.21444) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24614 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.11684) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01149 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.88219) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60742 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.47812) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32129 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.19199) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13441 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.00511) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34578 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.21649) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58266 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.45336) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54399 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.41469) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09800 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.96870) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07348 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.94418) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07783 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.94853) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32505 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.19575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34611 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.21681) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24742 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.11812) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29297 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.16367) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77962 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.65032) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23415 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-2.10486) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.35674 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.22744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.24722 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.11792) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04136 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-1.91206) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93195 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-1.80265) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68038 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.55108) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09832 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.96902) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94476 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.81546) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90509 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.77579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22041 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.09111) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05461 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.92531) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78893 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.65963) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62642 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.49712) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67004 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.54074) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74814 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.61884) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83579 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.70649) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65930 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.53000) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66422 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.53492) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66145 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.53215) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56365 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.43435) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54993 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.42063) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37273 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.24343) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85040 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.72110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89674 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.76744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01250 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.88320) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97487 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.84557) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74632 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.61702) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69881 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.56951) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89203 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.76274) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69040 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.56110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78904 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.65974) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93285 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.80355) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91682 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.78752) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93250 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.80320) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67263 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.54333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63494 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.50564) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53597 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.40667) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75138 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.62208) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58686 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.45756) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38982 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.26052) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72319 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.59389) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54014 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.41084) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66871 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.53941) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51684 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.38754) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.19053 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.06123) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83998 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.71068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67021 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.54091) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78109 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.65179) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80226 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.67296) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79862 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.66932) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92896 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.79966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65549 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.52619) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63900 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.50970) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49576 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.36646) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80441 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.67511) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68595 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.55665) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62231 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.49301) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63306 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.50376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29468 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.16538) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52873 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.39943) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23212 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.10282) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29890 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.16960) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37640 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.24710) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61632 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.48702) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31161 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.18231) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45947 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.33017) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57882 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.44952) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52976 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.40046) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37436 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.24506) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34829 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.21899) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25718 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-1.12788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34007 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.21077) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45768 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.32838) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46383 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.33453) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35868 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.22938) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25188 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.12258) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02502 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.89572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12330 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.99400) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47542 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.34612) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12732 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.99802) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02479 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.89549) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10637 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.97707) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06708 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.93778) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96196 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.83266) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85869 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.72939) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84928 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.71998) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83616 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.70686) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90462 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.77533) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95263 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.82333) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04577 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.91647) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94343 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.81413) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95965 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.83035) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17807 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-2.04877) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99682 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.86752) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94112 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.81182) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98000 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.85070) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08808 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.95878) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76895 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.63965) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90936 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.78006) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87328 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.74398) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02574 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.89644) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06781 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.93851) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91287 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.78357) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96253 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.83323) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17081 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-2.04151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89730 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.76801) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04615 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.91685) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92560 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.79631) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05187 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.92257) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92419 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.79489) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04642 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.91712) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71798 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.58868) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82718 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.69788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93652 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-1.80722) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94952 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.82022) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61316 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-1.48386) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56701 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-1.43771) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61676 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-1.48746) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59020 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-1.46090) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07905 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.94975) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22137 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-2.09207) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.11752 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-2.98822) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82732 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.69802) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99075 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.86145) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07110 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.94180) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87559 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.74629) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.05181 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.92251) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08925 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.95995) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11638 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.98708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78680 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.65750) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74435 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.61505) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90979 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.78050) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84672 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.71742) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59256 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.46327) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61004 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.48074) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46795 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.33865) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64588 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.51658) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54245 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.41315) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37834 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.24904) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.27918 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.14988) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41306 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.28376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68768 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.55838) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94980 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.82050) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17712 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-2.04782) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64443 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.51513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56278 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.43348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62229 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.49299) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31319 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.18389) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.24130 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.11200) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56572 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.43642) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45466 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.32536) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13437 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-2.00507) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59020 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.46090) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33109 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.20179) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82776 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.69846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65328 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.52398) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80474 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.67544) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79794 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.66864) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99715 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.86785) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57146 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.44216) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62155 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.49225) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74134 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.61204) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52517 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.39587) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55880 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.42950) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68134 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.55204) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76335 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.63405) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36498 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.23568) | 1 | 1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44378 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.31448) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57720 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.44790) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66379 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.53449) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83287 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.70357) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88960 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.76030) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68106 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.55176) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72357 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.59427) | -1 | -1 |
| G: -5278.76361 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73873 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.60943) | -1 | -1 |