乙二醇作为反应物的反应表19-10

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: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61162 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.81270) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.87264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.07372) | 1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68438 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.88546) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58337 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.78445) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62568 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.82676) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76441 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.96549) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.08188 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.28296) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.95783 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.15891) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55221 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.75329) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53670 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.73778) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65687 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.85795) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56100 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.76208) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42658 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.62766) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.99609 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.19716) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.22252 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.42360) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.92441 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.12549) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53436 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.73544) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39014 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.59122) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.69656 HOMO: -6.58788 LUMO: 1.73881 factor:1 | -1 (1.10236) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56693 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.76801) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09874 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.29982) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35777 HOMO: -6.80829 LUMO: 2.45991 factor:1 | -1 (0.44115) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42176 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.62284) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25743 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.45851) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26493 HOMO: -6.26134 LUMO: 1.46125 factor:1 | -1 (1.53399) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26485 HOMO: -7.54028 LUMO: 0.25851 factor:1 | -1 (1.53407) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24997 HOMO: -6.97700 LUMO: -0.73471 factor:1 | -1 (1.54895) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83655 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.03763) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.65806 HOMO: -6.83550 LUMO: -0.56872 factor:1 | -1 (1.14086) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.54331 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (1.25561) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14556 HOMO: -6.73482 LUMO: 1.89935 factor:1 | -1 (1.65336) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67897 HOMO: -6.61781 LUMO: 1.86670 factor:1 | -1 (0.11995) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.48103 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.68211) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.03614 HOMO: -7.23551 LUMO: 2.09800 factor:1 | -1 (1.76278) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44304 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.64412) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.12308 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-1.32416) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.70993 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.91101) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.72909 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.93017) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68472 HOMO: -6.39740 LUMO: 2.59597 factor:1 | -1 (1.11420) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41803 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.61911) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.49628 HOMO: -7.11306 LUMO: 0.90614 factor:1 | -1 (1.30264) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31587 HOMO: -6.61781 LUMO: -2.46263 factor:1 | -1 (1.48305) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.33268 HOMO: -6.96611 LUMO: 0.90614 factor:1 | -1 (0.46624) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15117 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.35225) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.40530 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.60638) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.12385 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.32493) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.88084 HOMO: -7.14299 LUMO: 0.98777 factor:1 | -1 (0.91808) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53804 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.73912) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42813 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.62921) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34113 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.54221) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41009 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.61117) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67355 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.87463) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68454 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.88562) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.21233 HOMO: -6.40556 LUMO: -0.42722 factor:1 | -1 (1.58659) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08428 HOMO: -7.18653 LUMO: 0.42178 factor:1 | -1 (1.71464) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51642 HOMO: -6.63958 LUMO: -0.71294 factor:1 | -1 (1.28250) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08297 HOMO: -6.63958 LUMO: -0.71022 factor:1 | -1 (1.71595) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18143 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.38251) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35853 HOMO: -6.56883 LUMO: -0.80274 factor:1 | -1 (0.44039) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62684 HOMO: -6.68584 LUMO: -0.56872 factor:1 | -1 (0.17208) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09754 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.29862) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32388 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.52496) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36119 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.56227) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.85696 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.05804) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49608 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.69716) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.48149 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.68257) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18772 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.38880) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53210 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.73318) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67657 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.87765) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67774 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.87882) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.63069 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.83177) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24949 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.45057) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64668 HOMO: -6.53073 LUMO: -0.74287 factor:1 | -1 (1.15224) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38413 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.58521) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35359 HOMO: -6.49264 LUMO: -0.44627 factor:1 | -1 (1.44533) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.23135 HOMO: -7.32803 LUMO: 0.41361 factor:1 | -1 (1.56757) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32649 HOMO: -6.53073 LUMO: -0.52790 factor:1 | -1 (1.47244) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48954 HOMO: -6.54978 LUMO: -0.53062 factor:1 | -1 (1.30938) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29084 HOMO: -6.56611 LUMO: -0.37824 factor:1 | -1 (1.50808) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15773 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.35881) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.97028 HOMO: -7.08040 LUMO: 0.45715 factor:1 | -1 (0.82864) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41988 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.62096) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06644 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.26752) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.05300 HOMO: -6.53345 LUMO: -0.29660 factor:1 | -1 (0.74592) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.04434 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.24542) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55898 HOMO: -6.98788 LUMO: 2.01092 factor:1 | -1 (1.23994) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30455 HOMO: -6.61781 LUMO: 1.92384 factor:1 | -1 (1.49437) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.44524 HOMO: -6.61237 LUMO: 2.06807 factor:1 | -1 (1.35368) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.54434 HOMO: -6.59060 LUMO: 1.95106 factor:1 | -1 (1.25458) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55294 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (1.24598) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26496 HOMO: -6.84911 LUMO: 2.03541 factor:1 | -1 (1.53396) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22463 HOMO: -6.50624 LUMO: 2.17147 factor:1 | -1 (1.57429) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.44047 HOMO: -6.68312 LUMO: 2.08439 factor:1 | -1 (1.35845) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.70712 HOMO: -6.96067 LUMO: 1.98099 factor:1 | -1 (1.09180) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39577 HOMO: -6.93618 LUMO: 1.85854 factor:1 | -1 (1.40316) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.21307 HOMO: -6.71305 LUMO: -0.61226 factor:1 | -1 (1.58585) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52173 HOMO: -7.06408 LUMO: 0.80001 factor:1 | -1 (1.27719) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55033 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (1.24859) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29473 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (1.50419) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.10722 HOMO: -6.85455 LUMO: 0.84900 factor:1 | -1 (1.69170) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.75666 HOMO: -6.60148 LUMO: -0.78369 factor:1 | -1 (0.04226) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57504 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-0.77612) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61004 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.81112) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.97998 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.18106) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.84523 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.04631) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.96039 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.16147) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62258 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.82366) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.08904 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.29012) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.69963 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.09929) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58046 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.78154) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38449 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.41443) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.91990 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.12098) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41265 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-0.61373) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30617 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.50725) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.60882 HOMO: -6.63958 LUMO: 0.57416 factor:1 | -1 (0.19010) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.34457 HOMO: -6.37563 LUMO: -0.48164 factor:1 | -1 (0.45435) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.02252 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-0.22360) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14652 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-0.34760) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.91609 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.11717) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.56409 HOMO: -6.77019 LUMO: -1.03131 factor:1 | -1 (1.23483) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26286 HOMO: -6.80285 LUMO: 1.05852 factor:1 | -1 (1.53606) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68263 HOMO: -6.76475 LUMO: 1.01771 factor:1 | -1 (1.11629) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20256 HOMO: -6.92530 LUMO: 1.37417 factor:1 | -1 (1.59636) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52451 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.72559) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49635 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.69743) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.45980 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.66088) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74994 HOMO: -6.78652 LUMO: 1.35785 factor:1 | -1 (0.04898) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04866 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-1.24974) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47738 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.67846) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44154 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.64262) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69083 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.89191) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67556 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.87664) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68786 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.88894) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.86804 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.06912) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30437 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.50545) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49009 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.69117) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38530 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.58638) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41104 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.61212) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.56643 HOMO: -6.72393 LUMO: -0.65307 factor:1 | -1 (0.23249) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29269 HOMO: -6.29671 LUMO: -0.39729 factor:1 | -1 (1.50623) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27100 HOMO: -6.75387 LUMO: -0.53334 factor:1 | -1 (1.52792) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.30884 HOMO: -6.53073 LUMO: -0.31293 factor:1 | -1 (0.49008) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19597 HOMO: -6.42189 LUMO: -0.59049 factor:1 | -1 (0.60295) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04721 HOMO: -6.41100 LUMO: -0.29933 factor:1 | -1 (0.75171) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14021 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.34129) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31145 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.51253) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06766 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.26874) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25572 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.45680) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.50150 HOMO: -6.32665 LUMO: -0.41906 factor:1 | -1 (0.29742) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.40873 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.60981) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09313 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.29421) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.25692 HOMO: -6.86271 LUMO: 2.07351 factor:1 | -1 (0.54200) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14374 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.34482) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31537 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.51644) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.73173 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.93281) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95324 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.15432) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41841 HOMO: -6.06814 LUMO: 1.94561 factor:1 | -1 (1.38052) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19198 HOMO: -6.58788 LUMO: 2.01908 factor:1 | -1 (1.60694) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28999 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (1.50893) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47207 HOMO: -6.54434 LUMO: -0.42994 factor:1 | -1 (1.32685) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08558 HOMO: -6.94707 LUMO: 0.42994 factor:1 | -1 (1.71334) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.79638 HOMO: -6.98516 LUMO: 0.41361 factor:1 | -1 (2.00254) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.17715 HOMO: -6.31304 LUMO: -0.54967 factor:1 | -1 (1.62177) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37071 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.57179) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49172 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.69280) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.21193 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.41301) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56503 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.76611) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51273 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.71381) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56057 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.76165) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.88159 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.08267) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25028 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-0.45136) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94555 HOMO: -6.63958 LUMO: -0.67484 factor:1 | -1 (1.85337) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27889 HOMO: -7.08584 LUMO: 0.46259 factor:1 | -1 (1.52003) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.16248 HOMO: -6.80285 LUMO: -0.73199 factor:1 | -1 (1.63644) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.36833 HOMO: -6.44366 LUMO: -0.45443 factor:1 | -1 (0.43059) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.00126 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.20234) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19985 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.40093) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23588 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.43696) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37948 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.58055) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46722 HOMO: -6.56883 LUMO: 1.70615 factor:1 | -1 (1.33170) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67479 HOMO: -6.77836 LUMO: 1.77962 factor:1 | -1 (1.12413) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39745 HOMO: -6.38923 LUMO: 1.85854 factor:1 | -1 (1.40147) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67104 HOMO: -6.35658 LUMO: 2.16875 factor:1 | -1 (1.12788) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.56456 HOMO: -6.83006 LUMO: 2.31025 factor:1 | -1 (1.23436) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31976 HOMO: -6.87087 LUMO: 1.79051 factor:1 | -1 (1.47916) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.11715 HOMO: -6.56339 LUMO: 2.37828 factor:1 | -1 (1.68177) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62412 HOMO: -6.30488 LUMO: 2.51705 factor:1 | -1 (1.17480) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68358 HOMO: -6.69400 LUMO: 1.95650 factor:1 | -1 (1.11534) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.40676 HOMO: -6.51168 LUMO: 2.03541 factor:1 | -1 (1.39216) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55539 HOMO: -6.30760 LUMO: 1.65173 factor:1 | -1 (1.24353) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94974 HOMO: -6.55250 LUMO: 1.90752 factor:1 | -1 (1.84918) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57335 HOMO: -6.41372 LUMO: 1.76058 factor:1 | -1 (1.22557) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19269 HOMO: -6.23957 LUMO: 2.06534 factor:1 | -1 (1.60623) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.12553 HOMO: -6.58243 LUMO: 2.11705 factor:1 | -1 (1.67339) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55664 HOMO: -6.37835 LUMO: 2.09256 factor:1 | -1 (1.24228) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.04757 HOMO: -6.50624 LUMO: 2.55787 factor:1 | -1 (1.75135) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57582 HOMO: -6.45454 LUMO: 1.87214 factor:1 | -1 (1.22310) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51601 HOMO: -6.53617 LUMO: 1.95650 factor:1 | -1 (1.28291) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14822 HOMO: -6.51985 LUMO: 1.71432 factor:1 | -1 (1.65070) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.59629 HOMO: -6.75114 LUMO: 1.84493 factor:1 | -1 (1.20263) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43081 HOMO: -6.06270 LUMO: 1.65717 factor:1 | -1 (1.36811) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62611 HOMO: -5.89671 LUMO: 1.71704 factor:1 | -1 (1.17281) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26967 HOMO: -6.18787 LUMO: 1.91840 factor:1 | -1 (1.52925) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48170 HOMO: -6.01644 LUMO: 1.85582 factor:1 | -1 (1.31722) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.61874 HOMO: -6.05998 LUMO: 2.33474 factor:1 | -1 (1.18019) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14752 HOMO: -6.05725 LUMO: 2.03541 factor:1 | -1 (1.65140) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.99837 HOMO: -6.80829 LUMO: 1.90480 factor:1 | -1 (1.80055) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.06108 HOMO: -6.76475 LUMO: 2.20956 factor:1 | -1 (0.73784) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.00476 HOMO: -6.29944 LUMO: 1.77962 factor:1 | -1 (0.79416) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92383 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (0.87509) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.18699 HOMO: -6.57699 LUMO: -0.47348 factor:1 | -1 (0.61193) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.43059 HOMO: -7.20830 LUMO: 0.49797 factor:1 | -1 (0.36833) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.31657 HOMO: -7.49402 LUMO: 0.29933 factor:1 | -1 (0.48235) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.49355 HOMO: -6.66679 LUMO: -0.58777 factor:1 | -1 (0.30537) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19447 HOMO: -6.67767 LUMO: -0.56328 factor:1 | -1 (0.60445) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35453 HOMO: -7.42871 LUMO: 0.35647 factor:1 | -1 (0.44439) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.98459 HOMO: -6.56067 LUMO: -0.54423 factor:1 | -1 (0.81433) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04848 HOMO: -6.56339 LUMO: -0.50341 factor:1 | -1 (0.75044) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.33829 HOMO: -6.56067 LUMO: -0.48436 factor:1 | -1 (0.46063) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.30035 HOMO: -6.73210 LUMO: 1.75241 factor:1 | -1 (0.49857) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76422 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.96530) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.93302 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.13410) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18410 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.38518) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74061 HOMO: -6.40828 LUMO: 2.10072 factor:1 | -1 (0.05831) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49031 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.69139) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36647 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.56755) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68800 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.88908) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73375 HOMO: -6.61509 LUMO: 2.11160 factor:1 | -1 (0.06517) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62779 HOMO: -6.82734 LUMO: 1.77146 factor:1 | -1 (0.17113) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.88137 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-0.08245) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24655 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.44763) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.82457 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.02565) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55197 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.75305) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83835 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.03943) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76843 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.96951) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.18401 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.38509) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89402 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.09510) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14861 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.34969) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.03084 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.23192) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.12150 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-1.32258) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.28664 HOMO: -6.53890 LUMO: 1.92929 factor:1 | -1 (0.51228) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39912 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.60020) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38893 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (0.40999) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.94386 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.85506) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.29379 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-0.49487) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62319 HOMO: -6.29944 LUMO: 1.90208 factor:1 | -1 (0.17573) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.98365 HOMO: -6.75114 LUMO: 1.85854 factor:1 | -1 (1.81527) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33615 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.53723) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68405 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.88513) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71654 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.91762) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49548 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.69656) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.60057 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.80165) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.60167 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (1.19725) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30573 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.50681) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.59365 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (1.20527) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38488 HOMO: -6.84094 LUMO: -1.37690 factor:1 | -1 (1.41404) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09523 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.29630) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95392 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.15500) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.20558 HOMO: -7.21102 LUMO: 0.82995 factor:1 | -1 (0.59334) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.20203 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.40311) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34522 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.54630) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73906 HOMO: -6.83550 LUMO: -0.98777 factor:1 | -1 (0.05987) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.60095 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.80203) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32301 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.52409) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69281 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.89389) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19814 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.39922) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.40414 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (0.39478) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44046 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.64154) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34383 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.54491) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19060 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.39168) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.53113 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (0.26779) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.32476 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (0.47416) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.06827 HOMO: -7.00965 LUMO: 0.82995 factor:1 | -1 (0.73065) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01449 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.21557) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.82366 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.02474) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57909 HOMO: -6.60420 LUMO: -0.53334 factor:1 | -1 (1.21983) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.23514 HOMO: -6.78652 LUMO: -0.79729 factor:1 | -1 (1.56378) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47269 HOMO: -6.48992 LUMO: -0.64491 factor:1 | -1 (1.32623) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14792 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (1.65100) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.91426 HOMO: -6.65046 LUMO: -0.78097 factor:1 | -1 (1.88466) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34885 HOMO: -7.24095 LUMO: 0.37280 factor:1 | -1 (1.45007) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.97002 HOMO: -6.81101 LUMO: -0.74831 factor:1 | -1 (1.82890) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.10862 HOMO: -6.69400 LUMO: -0.77280 factor:1 | -1 (0.69030) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92878 HOMO: -6.08447 LUMO: -0.68573 factor:1 | -1 (0.87014) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53336 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.73444) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47140 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.67247) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51300 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.71408) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83293 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.03401) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.18760 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-1.38868) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.72884 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.92992) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69281 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-0.89389) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24383 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.44491) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61417 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.81525) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56182 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.76290) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.40931 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.38961) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43920 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.64028) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32971 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.53079) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38865 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.58973) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.58934 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.20958) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.81505 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (1.98387) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15601 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (1.64291) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.31684 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (0.48208) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04348 HOMO: -7.18925 LUMO: -0.63130 factor:1 | -1 (0.75544) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11738 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.31845) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36358 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.56466) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25898 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.46006) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95533 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.15641) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11825 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.31933) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92440 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (0.87452) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.71588 HOMO: -6.80829 LUMO: -0.59865 factor:1 | -1 (1.08304) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12432 HOMO: -6.63686 LUMO: -0.75103 factor:1 | -1 (0.67460) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.79319 HOMO: -6.73210 LUMO: -0.55511 factor:1 | -1 (1.00573) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.56346 HOMO: -6.50624 LUMO: 1.58642 factor:1 | -1 (0.23546) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59445 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.79552) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47972 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.68080) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46821 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.66929) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25349 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.45457) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.64441 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.84548) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53518 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.73626) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44671 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.64779) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26641 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.46749) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31583 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.51691) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52927 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.73035) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43237 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.63345) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28687 HOMO: -7.00149 LUMO: 0.99866 factor:1 | -1 (1.51206) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.05336 HOMO: -7.13755 LUMO: 1.05308 factor:1 | -1 (1.74556) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.02596 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (1.77296) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.77959 HOMO: -6.63141 LUMO: -0.88981 factor:1 | -1 (2.01933) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.89603 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (1.90289) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20433 HOMO: -6.55794 LUMO: -0.80818 factor:1 | -1 (1.59459) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.07092 HOMO: -6.95251 LUMO: -0.97145 factor:1 | -1 (1.72800) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.20140 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.40248) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06317 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.26425) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26160 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.46268) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.87621 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (0.92271) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15430 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.35538) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43288 HOMO: -6.55794 LUMO: -0.54967 factor:1 | -1 (1.36604) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24520 HOMO: -6.71577 LUMO: -0.53879 factor:1 | -1 (1.55372) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51188 HOMO: -6.88992 LUMO: -0.55511 factor:1 | -1 (1.28704) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26869 HOMO: -6.74026 LUMO: -0.60681 factor:1 | -1 (1.53023) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50124 HOMO: -6.76747 LUMO: -0.50885 factor:1 | -1 (1.29768) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29979 HOMO: -6.87904 LUMO: -0.92519 factor:1 | -1 (1.49913) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.96006 HOMO: -6.53073 LUMO: -0.53062 factor:1 | -1 (1.83886) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32202 HOMO: -6.97700 LUMO: -0.98505 factor:1 | -1 (1.47690) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37212 HOMO: -6.96884 LUMO: -0.79185 factor:1 | -1 (1.42680) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35772 HOMO: -6.60420 LUMO: -0.31021 factor:1 | -1 (1.44120) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.13410 HOMO: -6.68584 LUMO: -0.63947 factor:1 | -1 (1.66482) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.96008 HOMO: -6.41917 LUMO: -0.35103 factor:1 | -1 (1.83884) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30159 HOMO: -6.73482 LUMO: -0.70477 factor:1 | -1 (1.49733) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15775 HOMO: -6.71305 LUMO: -0.85716 factor:1 | -1 (1.64117) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.97652 HOMO: -6.70761 LUMO: -0.63403 factor:1 | -1 (1.82240) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.73886 HOMO: -6.37563 LUMO: -0.38640 factor:1 | -1 (2.06007) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38521 HOMO: -6.27495 LUMO: -0.54967 factor:1 | -1 (1.41371) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20025 HOMO: -6.98516 LUMO: 0.38096 factor:1 | -1 (1.59867) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51729 HOMO: -6.47087 LUMO: -0.40001 factor:1 | -1 (1.28163) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43275 HOMO: -6.59876 LUMO: 0.20681 factor:1 | -1 (1.36617) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.05132 HOMO: -6.89809 LUMO: 0.14966 factor:1 | -1 (1.74760) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29574 HOMO: -6.76203 LUMO: 2.11432 factor:1 | -1 (1.50318) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46749 HOMO: -6.58516 LUMO: 1.75786 factor:1 | -1 (1.33143) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22316 HOMO: -6.37835 LUMO: 1.84493 factor:1 | -1 (1.57576) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27424 HOMO: -6.83550 LUMO: 1.74425 factor:1 | -1 (1.52468) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47291 HOMO: -6.65318 LUMO: 1.79051 factor:1 | -1 (1.32601) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34597 HOMO: -6.68584 LUMO: 2.11160 factor:1 | -1 (1.45295) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.89325 HOMO: -6.36202 LUMO: 1.85037 factor:1 | -1 (1.90567) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.09380 HOMO: -6.68312 LUMO: 2.23133 factor:1 | -1 (1.70512) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.85045 HOMO: -6.66679 LUMO: 2.14154 factor:1 | -1 (1.94847) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.11097 HOMO: -6.50896 LUMO: 1.92657 factor:1 | -1 (1.68795) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35465 HOMO: -6.63686 LUMO: 2.22317 factor:1 | -1 (1.44427) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.95591 HOMO: -6.58788 LUMO: 2.17419 factor:1 | -1 (0.84301) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74014 HOMO: -6.72665 LUMO: 2.12249 factor:1 | -1 (0.05878) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.26024 HOMO: -6.28311 LUMO: 1.91024 factor:1 | -1 (0.53868) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.41763 HOMO: -6.56067 LUMO: 2.27487 factor:1 | -1 (0.38129) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46803 HOMO: -6.83006 LUMO: 2.28031 factor:1 | -1 (0.33089) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.49584 HOMO: -6.45182 LUMO: 1.62724 factor:1 | -1 (0.30308) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.32631 HOMO: -6.78380 LUMO: 1.83677 factor:1 | -1 (0.47261) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51570 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.71678) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67608 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.87716) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57121 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.77229) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.78362 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.98470) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.86058 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.06166) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11484 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.31592) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.94105 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.14213) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49817 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.69925) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47295 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.67403) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.04676 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.24784) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.05045 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.25153) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.27253 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.47361) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04256 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.24364) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44144 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.64252) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26766 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.46874) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41890 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.61998) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.35528 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.55636) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67859 HOMO: -6.40828 LUMO: 2.05174 factor:1 | -1 (0.12033) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.45069 HOMO: -6.60420 LUMO: -0.82450 factor:1 | -1 (2.34823) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46514 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.66622) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67230 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.87338) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71336 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.91444) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.54356 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.74464) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53850 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.73958) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.66875 HOMO: -6.74842 LUMO: -0.51974 factor:1 | -1 (1.13017) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46587 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.66695) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15931 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.36039) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44979 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.65087) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24804 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.44912) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89304 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.09412) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30131 HOMO: -6.84638 LUMO: 0.24762 factor:1 | -1 (1.49761) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41724 HOMO: -6.66951 LUMO: 0.39184 factor:1 | -1 (1.38169) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15707 HOMO: -6.62597 LUMO: -0.65035 factor:1 | -1 (1.64185) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34961 HOMO: -7.13755 LUMO: 0.45715 factor:1 | -1 (1.44931) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.22189 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.42297) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23613 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-0.43721) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.94731 HOMO: -6.36202 LUMO: -0.29660 factor:1 | -1 (0.85161) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01408 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.21516) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.74342 HOMO: -6.70761 LUMO: 0.41906 factor:1 | -1 (1.05550) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.05237 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.25345) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89816 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.09924) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37231 HOMO: -7.19741 LUMO: -1.00954 factor:1 | -1 (1.42661) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20733 HOMO: -6.58243 LUMO: -0.33470 factor:1 | -1 (1.59159) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37326 HOMO: -7.22190 LUMO: 0.49253 factor:1 | -1 (1.42566) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22923 HOMO: -7.22462 LUMO: 0.51974 factor:1 | -1 (1.56969) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.12586 HOMO: -7.08584 LUMO: -0.68301 factor:1 | -1 (1.67306) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29258 HOMO: -6.68584 LUMO: -0.29660 factor:1 | -1 (1.50634) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28594 HOMO: -6.33753 LUMO: -0.48436 factor:1 | -1 (1.51298) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.17886 HOMO: -7.15932 LUMO: 0.55511 factor:1 | -1 (1.62006) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.83344 HOMO: -6.57427 LUMO: 2.01908 factor:1 | -1 (1.96548) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37745 HOMO: -6.75659 LUMO: 2.22045 factor:1 | -1 (1.42147) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.04150 HOMO: -6.73482 LUMO: 2.20956 factor:1 | -1 (1.75742) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.41913 HOMO: -6.74026 LUMO: 1.76602 factor:1 | -1 (0.37979) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.34250 HOMO: -6.95523 LUMO: 1.94834 factor:1 | -1 (0.45642) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38153 HOMO: -6.33209 LUMO: 1.87486 factor:1 | -1 (0.41740) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.13766 HOMO: -6.71033 LUMO: 2.12521 factor:1 | -1 (0.66126) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.03140 HOMO: -6.50080 LUMO: 2.04902 factor:1 | -1 (0.76752) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.61606 HOMO: -6.76475 LUMO: 1.94017 factor:1 | -1 (0.18286) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38691 HOMO: -6.53073 LUMO: 2.08983 factor:1 | -1 (0.41201) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43918 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.64026) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30538 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.50646) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26391 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-0.46499) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.90719 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.10827) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73530 HOMO: -6.93346 LUMO: 1.79595 factor:1 | -1 (0.06362) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83691 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.03799) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.50375 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.70483) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.95500 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-1.15608) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21139 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.41247) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.23194 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (0.56698) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11463 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.31571) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46384 HOMO: -6.67767 LUMO: 2.43814 factor:1 | -1 (0.33508) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33074 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.53182) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37768 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.57876) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.16402 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.36510) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.57821 HOMO: -6.38379 LUMO: 1.68438 factor:1 | -1 (0.22071) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.29543 HOMO: -6.78924 LUMO: 2.01364 factor:1 | -1 (0.50349) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.97073 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.17181) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01830 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.21938) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.80493 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.00601) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.33568 HOMO: -6.67223 LUMO: 1.91840 factor:1 | -1 (1.46324) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31389 HOMO: -6.79196 LUMO: 2.18507 factor:1 | -1 (1.48503) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.99355 HOMO: -6.93346 LUMO: 1.78235 factor:1 | -1 (1.80537) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.10710 HOMO: -6.16882 LUMO: 1.80956 factor:1 | -1 (0.69182) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.95330 HOMO: -6.72665 LUMO: 2.07895 factor:1 | -1 (0.84562) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.01967 HOMO: -6.73210 LUMO: 1.97827 factor:1 | -1 (0.77925) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12699 HOMO: -6.84638 LUMO: 1.87214 factor:1 | -1 (0.67193) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.81077 HOMO: -6.83006 LUMO: 2.36195 factor:1 | -1 (0.98815) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.64784 HOMO: -6.97700 LUMO: 1.91024 factor:1 | -1 (0.15108) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46584 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.66692) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.06566 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-1.26674) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.45904 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.66012) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21640 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.41748) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55289 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.75397) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47444 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.67552) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52919 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.73027) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44258 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.64366) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46484 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.66592) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.64733 HOMO: -7.18108 LUMO: 2.10072 factor:1 | -1 (0.15159) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36598 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.56706) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31011 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.51119) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23841 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.43949) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.51946 HOMO: -6.45454 LUMO: 2.15786 factor:1 | -1 (0.27946) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49744 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.69852) | 1 | 1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.03171 HOMO: -6.93618 LUMO: 1.86942 factor:1 | -1 (2.76721) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.88248 HOMO: -6.63141 LUMO: 1.92657 factor:1 | -1 (1.91644) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.09143 HOMO: -6.51441 LUMO: -0.44355 factor:1 | -1 (1.70749) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94514 HOMO: -6.82734 LUMO: -1.03131 factor:1 | -1 (1.85378) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12536 HOMO: -6.58788 LUMO: -0.82995 factor:1 | -1 (0.67356) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19695 HOMO: -6.43277 LUMO: -0.40817 factor:1 | -1 (0.60197) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.97466 HOMO: -6.78924 LUMO: -0.72110 factor:1 | -1 (0.82426) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15983 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.36090) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.08899 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-0.29007) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.96973 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-0.17081) | -1 | -1 |
| G: -5750.43323 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15792 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-0.35900) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.72478 HOMO: -6.79740 LUMO: -0.79185 factor:1 | -1 (1.06397) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27470 HOMO: -6.08719 LUMO: -0.63675 factor:1 | -1 (1.51404) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53392 HOMO: -6.84094 LUMO: 0.42994 factor:1 | -1 (1.25483) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38314 HOMO: -6.59604 LUMO: 0.25851 factor:1 | -1 (1.40560) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67523 HOMO: -6.82462 LUMO: 0.08708 factor:1 | -1 (1.11352) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.25584 HOMO: -6.54706 LUMO: 0.44082 factor:1 | -1 (1.53290) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45228 HOMO: -6.99333 LUMO: 0.32109 factor:1 | -1 (1.33646) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62703 HOMO: -6.29944 LUMO: -0.57144 factor:1 | -1 (1.16171) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41432 HOMO: -6.57699 LUMO: -0.46531 factor:1 | -1 (1.37442) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48197 HOMO: -6.24773 LUMO: -0.53879 factor:1 | -1 (1.30677) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48154 HOMO: -6.96067 LUMO: -0.67212 factor:1 | -1 (1.30721) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64913 HOMO: -7.24095 LUMO: -0.09252 factor:1 | -1 (1.13961) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.36485 HOMO: -6.33481 LUMO: -0.46531 factor:1 | -1 (1.42389) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46766 HOMO: -6.43549 LUMO: -0.33198 factor:1 | -1 (1.32109) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28654 HOMO: -6.53073 LUMO: 0.44899 factor:1 | -1 (1.50220) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39171 HOMO: -6.69128 LUMO: 0.47620 factor:1 | -1 (1.39703) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26161 HOMO: -6.65318 LUMO: 0.52246 factor:1 | -1 (1.52713) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.42088 HOMO: -6.71305 LUMO: 0.41089 factor:1 | -1 (1.36786) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.18512 HOMO: -6.70216 LUMO: 0.19864 factor:1 | -1 (1.60362) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29250 HOMO: -6.41100 LUMO: 0.34558 factor:1 | -1 (1.49625) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.49680 HOMO: -7.01237 LUMO: 0.02993 factor:1 | -1 (1.29194) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.10254 HOMO: -6.85999 LUMO: 0.18776 factor:1 | -1 (1.68621) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38031 HOMO: -6.62869 LUMO: 0.48708 factor:1 | -1 (1.40843) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53158 HOMO: -6.43821 LUMO: -0.45715 factor:1 | -1 (1.25717) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43694 HOMO: -6.43277 LUMO: -0.72110 factor:1 | -1 (1.35181) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.25133 HOMO: -7.10761 LUMO: 0.43266 factor:1 | -1 (1.53742) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.36219 HOMO: -6.57699 LUMO: -0.61498 factor:1 | -1 (1.42656) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53196 HOMO: -6.82189 LUMO: -0.75648 factor:1 | -1 (1.25679) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52758 HOMO: -6.55794 LUMO: -0.67212 factor:1 | -1 (1.26117) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32118 HOMO: -6.69128 LUMO: 1.88575 factor:1 | -1 (1.46756) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22496 HOMO: -6.65591 LUMO: 1.70888 factor:1 | -1 (1.56378) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.33849 HOMO: -6.58788 LUMO: 1.68438 factor:1 | -1 (1.45026) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45334 HOMO: -6.46270 LUMO: 1.72520 factor:1 | -1 (1.33540) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39250 HOMO: -6.57427 LUMO: 1.73881 factor:1 | -1 (1.39624) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19067 HOMO: -6.45182 LUMO: 1.75241 factor:1 | -1 (1.59807) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.40246 HOMO: -6.51441 LUMO: 1.78779 factor:1 | -1 (1.38628) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31742 HOMO: -6.67495 LUMO: 2.11705 factor:1 | -1 (1.47132) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41990 HOMO: -6.22597 LUMO: 1.96466 factor:1 | -1 (1.36884) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34747 HOMO: -6.68040 LUMO: 2.30753 factor:1 | -1 (1.44128) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.97879 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.19004) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76746 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.97871) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.10610 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-1.31736) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.50827 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.71952) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57760 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.78886) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71679 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.92804) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.74005 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.95131) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.81333 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.02459) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.70209 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.91335) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56625 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.77751) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65711 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.86837) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39801 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.60926) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.93449 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.14574) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59700 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.80826) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69872 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.90998) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62909 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.84034) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55798 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.76924) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.13395 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.34520) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52439 HOMO: -6.35658 LUMO: 2.16603 factor:1 | -1 (1.26435) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21857 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.42983) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.50041 HOMO: -6.35114 LUMO: 2.10616 factor:1 | -1 (0.28833) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11830 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.32956) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50605 HOMO: -6.24773 LUMO: 1.98915 factor:1 | -1 (1.28269) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26096 HOMO: -6.53617 LUMO: 2.42726 factor:1 | -1 (1.52778) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.65618 HOMO: -6.59332 LUMO: 1.82316 factor:1 | -1 (1.13257) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.15617 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.36743) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68604 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.89730) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65379 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.86505) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18143 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.39269) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37549 HOMO: -6.24773 LUMO: 2.12793 factor:1 | -1 (1.41325) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62130 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.83256) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65249 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.86374) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.66841 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.87966) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01816 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.22942) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50254 HOMO: -6.15794 LUMO: 2.00548 factor:1 | -1 (1.28620) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35767 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (1.43107) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32013 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.53138) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.27264 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.48390) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92671 HOMO: -6.76747 LUMO: 2.20956 factor:1 | -1 (0.86203) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64287 HOMO: -6.14161 LUMO: 1.80684 factor:1 | -1 (1.14587) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57381 HOMO: -6.81373 LUMO: 1.91024 factor:1 | -1 (1.21493) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.76135 HOMO: -6.81917 LUMO: 2.34834 factor:1 | -1 (1.02739) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.69727 HOMO: -6.72121 LUMO: 1.90208 factor:1 | -1 (1.09148) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.75306 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.96432) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61937 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.83063) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.90806 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.11931) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.47353 HOMO: -6.80557 LUMO: -0.60954 factor:1 | -1 (0.31522) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43379 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-0.64505) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65026 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.86151) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71921 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.93047) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58949 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.80075) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44750 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-0.65876) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45511 HOMO: -6.61781 LUMO: -0.69661 factor:1 | -1 (1.33363) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65053 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.86178) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68419 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.89545) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.35371 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.56496) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68320 HOMO: -6.80285 LUMO: -0.52246 factor:1 | -1 (1.10554) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51316 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.72442) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.21194 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.57680) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55844 HOMO: -6.71849 LUMO: -0.48164 factor:1 | -1 (1.23031) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18780 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.39905) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04093 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-1.25219) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46095 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.67220) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46957 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.68083) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59330 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.80456) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55651 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.76777) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56204 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.77329) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65573 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-0.86698) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61371 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.82497) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.90211 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.11336) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26551 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.47677) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24624 HOMO: -7.37429 LUMO: 0.09252 factor:1 | -1 (1.54250) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24274 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.45399) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32878 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-0.54004) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53849 HOMO: -6.95523 LUMO: -0.86804 factor:1 | -1 (1.25025) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21569 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-0.42695) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47529 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.68654) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67944 HOMO: -6.37835 LUMO: -0.53606 factor:1 | -1 (0.10931) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.44691 HOMO: -6.71849 LUMO: -0.61226 factor:1 | -1 (0.34183) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46422 HOMO: -6.68584 LUMO: -1.11022 factor:1 | -1 (0.32452) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.36400 HOMO: -6.80285 LUMO: -0.79185 factor:1 | -1 (0.42474) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62740 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.83865) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36157 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.57283) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33474 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.54600) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09242 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.30368) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.28894 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.50020) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.25660 HOMO: -7.43959 LUMO: 0.30477 factor:1 | -1 (0.53215) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.54152 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-0.75278) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61162 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-0.82287) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.87264 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.08389) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68438 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.89564) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58337 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-0.79463) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62568 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.83694) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76441 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.97566) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.08188 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.29314) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.95783 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.16908) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55221 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.76347) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53670 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.74796) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65687 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.86812) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56100 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.77226) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42658 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.63783) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.99609 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-1.20734) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.22252 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.43378) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.92441 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.13567) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53436 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.74562) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39014 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.60140) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.69656 HOMO: -6.31576 LUMO: 2.03813 factor:1 | -1 (1.09218) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56693 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.77819) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09874 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.30999) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35777 HOMO: -6.78108 LUMO: 2.16875 factor:1 | -1 (0.43097) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42176 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.63302) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25743 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.46869) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26493 HOMO: -6.72665 LUMO: 2.09528 factor:1 | -1 (1.52381) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26485 HOMO: -6.86543 LUMO: 1.91568 factor:1 | -1 (1.52389) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24997 HOMO: -5.83956 LUMO: 1.89391 factor:1 | -1 (1.53878) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83655 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.04781) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.65806 HOMO: -6.07630 LUMO: 1.80956 factor:1 | -1 (1.13069) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.54331 HOMO: -6.43277 LUMO: 1.81772 factor:1 | -1 (1.24544) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14556 HOMO: -7.03959 LUMO: 1.78779 factor:1 | -1 (1.64319) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67897 HOMO: -6.72121 LUMO: 2.29664 factor:1 | -1 (0.10977) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.48103 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.69228) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.03614 HOMO: -6.63958 LUMO: 1.84221 factor:1 | -1 (1.75260) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44304 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.65430) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.12308 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-1.33434) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.70993 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.92119) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.72909 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.94034) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68472 HOMO: -6.11168 LUMO: 1.70071 factor:1 | -1 (1.10402) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41803 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.62929) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.49628 HOMO: -6.81101 LUMO: 1.63540 factor:1 | -1 (1.29246) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31587 HOMO: -6.80013 LUMO: 2.12249 factor:1 | -1 (1.47287) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.33268 HOMO: -6.48447 LUMO: 1.94561 factor:1 | -1 (0.45606) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15117 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.36243) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.40530 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.61656) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.12385 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.33511) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.88084 HOMO: -6.77564 LUMO: 1.81228 factor:1 | -1 (0.90791) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53804 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.74929) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.42813 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.63939) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34113 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.55239) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41009 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.62134) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67355 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.88481) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68454 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.89580) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.21233 HOMO: -6.59604 LUMO: 2.59325 factor:1 | -1 (1.57641) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08428 HOMO: -6.11712 LUMO: 2.02181 factor:1 | -1 (1.70447) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51642 HOMO: -6.63141 LUMO: 2.09256 factor:1 | -1 (1.27232) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08297 HOMO: -6.61781 LUMO: 1.86126 factor:1 | -1 (1.70577) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18143 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.39269) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35853 HOMO: -6.60420 LUMO: 1.54561 factor:1 | -1 (0.43021) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62684 HOMO: -6.52529 LUMO: 2.05174 factor:1 | -1 (0.16191) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09754 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.30879) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32388 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.53514) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36119 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.57245) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.85696 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.06822) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49608 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.70733) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.48149 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.69275) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18772 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.39897) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53210 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.74336) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67657 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.88783) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67774 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.88900) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.63069 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.84195) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24949 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.46074) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64668 HOMO: -6.62597 LUMO: 2.10344 factor:1 | -1 (1.14206) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38413 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.59539) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35359 HOMO: -6.48447 LUMO: 1.91840 factor:1 | -1 (1.43516) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.23135 HOMO: -6.41372 LUMO: 1.61364 factor:1 | -1 (1.55739) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32649 HOMO: -6.37291 LUMO: 1.79051 factor:1 | -1 (1.46226) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48954 HOMO: -6.13073 LUMO: 1.77962 factor:1 | -1 (1.29921) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29084 HOMO: -6.13073 LUMO: 1.98915 factor:1 | -1 (1.49791) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15773 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.36899) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.97028 HOMO: -6.87087 LUMO: -0.82995 factor:1 | -1 (0.81846) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41988 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.63114) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06644 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.27769) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.05300 HOMO: -6.65863 LUMO: 1.52656 factor:1 | -1 (0.73574) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.04434 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.25560) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55898 HOMO: -6.68584 LUMO: 0.94424 factor:1 | -1 (1.22976) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30455 HOMO: -6.58788 LUMO: 1.00138 factor:1 | -1 (1.48419) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.44524 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (1.34351) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.54434 HOMO: -6.67223 LUMO: 0.80274 factor:1 | -1 (1.24440) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55294 HOMO: -6.95251 LUMO: 0.90614 factor:1 | -1 (1.23581) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26496 HOMO: -7.19469 LUMO: 1.34152 factor:1 | -1 (1.52378) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22463 HOMO: -6.59332 LUMO: -0.76464 factor:1 | -1 (1.56411) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.44047 HOMO: -6.77564 LUMO: -0.90886 factor:1 | -1 (1.34827) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.70712 HOMO: -6.57971 LUMO: -0.41633 factor:1 | -1 (1.08163) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39577 HOMO: -6.68856 LUMO: -0.58232 factor:1 | -1 (1.39298) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.21307 HOMO: -6.87087 LUMO: -0.71022 factor:1 | -1 (1.57568) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52173 HOMO: -6.67767 LUMO: -0.74559 factor:1 | -1 (1.26702) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55033 HOMO: -6.68040 LUMO: -0.65307 factor:1 | -1 (1.23842) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29473 HOMO: -6.32937 LUMO: 0.80274 factor:1 | -1 (1.49401) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.10722 HOMO: -6.29671 LUMO: 0.82723 factor:1 | -1 (1.68153) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.75666 HOMO: -6.67767 LUMO: 0.59321 factor:1 | -1 (0.03208) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57504 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.78630) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61004 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.82129) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.97998 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-1.19123) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.84523 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.05649) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.96039 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.17165) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62258 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.83384) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.08904 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-1.30030) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.69963 HOMO: -6.61237 LUMO: -0.48980 factor:1 | -1 (0.08912) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58046 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.79172) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38449 HOMO: -6.88992 LUMO: -0.70205 factor:1 | -1 (0.40425) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.91990 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.13116) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41265 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.62390) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30617 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-0.51742) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.60882 HOMO: -6.55250 LUMO: -0.49797 factor:1 | -1 (0.17992) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.34457 HOMO: -6.50896 LUMO: -0.46804 factor:1 | -1 (0.44417) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.02252 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.23377) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14652 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.35778) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.91609 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.12735) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.56409 HOMO: -6.72665 LUMO: -0.55239 factor:1 | -1 (1.22465) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26286 HOMO: -7.05319 LUMO: -1.08573 factor:1 | -1 (1.52588) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68263 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (1.10612) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20256 HOMO: -6.76475 LUMO: -0.53879 factor:1 | -1 (1.58618) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52451 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.73577) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49635 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.70760) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.45980 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.67106) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74994 HOMO: -6.69400 LUMO: -0.62858 factor:1 | -1 (0.03880) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04866 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.25991) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47738 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.68864) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44154 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.65280) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69083 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.90208) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67556 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.88682) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68786 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.89912) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.86804 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.07929) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30437 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.51563) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49009 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.70135) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38530 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.59656) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41104 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.62230) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.56643 HOMO: -6.53890 LUMO: -0.68845 factor:1 | -1 (0.22232) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29269 HOMO: -6.56611 LUMO: -0.66396 factor:1 | -1 (1.49605) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27100 HOMO: -6.04909 LUMO: -0.59865 factor:1 | -1 (1.51774) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.30884 HOMO: -6.74842 LUMO: -0.77825 factor:1 | -1 (0.47990) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19597 HOMO: -6.82462 LUMO: -0.61498 factor:1 | -1 (0.59277) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04721 HOMO: -7.40694 LUMO: 0.32926 factor:1 | -1 (0.74154) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14021 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.35146) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31145 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.52270) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06766 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.27892) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25572 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.46697) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.50150 HOMO: -6.65863 LUMO: -0.28028 factor:1 | -1 (0.28724) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.40873 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.61998) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09313 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-0.30439) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.25692 HOMO: -6.73754 LUMO: -0.77825 factor:1 | -1 (0.53182) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14374 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.35500) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31537 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.52662) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.73173 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.94298) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95324 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.16449) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41841 HOMO: -6.52529 LUMO: 1.65989 factor:1 | -1 (1.37034) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19198 HOMO: -6.63686 LUMO: 1.64629 factor:1 | -1 (1.59676) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28999 HOMO: -6.49808 LUMO: 1.60003 factor:1 | -1 (1.49875) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47207 HOMO: -6.85183 LUMO: 1.96194 factor:1 | -1 (1.31668) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.08558 HOMO: -6.90081 LUMO: 1.82316 factor:1 | -1 (1.70316) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.79638 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (1.99236) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.17715 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (1.61159) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37071 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.58197) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49172 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-0.70298) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.21193 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.42318) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56503 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.77629) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51273 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.72399) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56057 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-0.77182) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.88159 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.09285) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25028 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-0.46153) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94555 HOMO: -6.41100 LUMO: 1.74697 factor:1 | -1 (1.84319) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27889 HOMO: -6.34297 LUMO: 1.55921 factor:1 | -1 (1.50985) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.16248 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (1.62626) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.36833 HOMO: -6.50896 LUMO: 2.02725 factor:1 | -1 (0.42042) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.00126 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.21252) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19985 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.41111) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23588 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.44714) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37948 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.59073) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46722 HOMO: -6.77564 LUMO: 2.38372 factor:1 | -1 (1.32152) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67479 HOMO: -6.18243 LUMO: 2.40821 factor:1 | -1 (1.11395) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39745 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (1.39129) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67104 HOMO: -6.74570 LUMO: 1.88303 factor:1 | -1 (1.11771) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.56456 HOMO: -6.29944 LUMO: 2.05174 factor:1 | -1 (1.22419) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31976 HOMO: -7.00693 LUMO: 2.16331 factor:1 | -1 (1.46898) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.11715 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (1.67160) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62412 HOMO: -6.72665 LUMO: 2.03813 factor:1 | -1 (1.16462) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68358 HOMO: -6.69944 LUMO: 2.36467 factor:1 | -1 (1.10516) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.40676 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (1.38198) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55539 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (1.23336) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94974 HOMO: -6.70489 LUMO: 2.20956 factor:1 | -1 (1.83900) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57335 HOMO: -6.94707 LUMO: 1.81500 factor:1 | -1 (1.21540) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19269 HOMO: -6.39468 LUMO: 1.79051 factor:1 | -1 (1.59606) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.12553 HOMO: -6.69128 LUMO: 2.03813 factor:1 | -1 (1.66321) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55664 HOMO: -6.55250 LUMO: 2.00548 factor:1 | -1 (1.23210) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.04757 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (1.74117) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57582 HOMO: -6.85727 LUMO: 1.70071 factor:1 | -1 (1.21292) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51601 HOMO: -6.71305 LUMO: 1.72520 factor:1 | -1 (1.27273) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14822 HOMO: -6.81101 LUMO: 2.15514 factor:1 | -1 (1.64052) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.59629 HOMO: -6.93618 LUMO: 1.75513 factor:1 | -1 (1.19246) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43081 HOMO: -6.63686 LUMO: 2.09800 factor:1 | -1 (1.35793) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62611 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (1.16263) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26967 HOMO: -6.37019 LUMO: 2.35923 factor:1 | -1 (1.51908) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48170 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (1.30704) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.61874 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (1.17001) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14752 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (1.64123) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.99837 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (1.79037) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.06108 HOMO: -6.72121 LUMO: 1.33608 factor:1 | -1 (0.72766) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.00476 HOMO: -6.89264 LUMO: 2.08983 factor:1 | -1 (0.78399) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92383 HOMO: -6.31032 LUMO: 2.24766 factor:1 | -1 (0.86491) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.18699 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (0.60175) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.43059 HOMO: -6.78108 LUMO: 2.15786 factor:1 | -1 (0.35816) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.31657 HOMO: -6.50896 LUMO: 2.15786 factor:1 | -1 (0.47217) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.49355 HOMO: -6.56067 LUMO: 2.24494 factor:1 | -1 (0.29519) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19447 HOMO: -6.72938 LUMO: 2.24494 factor:1 | -1 (0.59427) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.35453 HOMO: -6.40556 LUMO: 1.58642 factor:1 | -1 (0.43421) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.98459 HOMO: -6.63141 LUMO: 1.66262 factor:1 | -1 (0.80415) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04848 HOMO: -6.97156 LUMO: 2.23678 factor:1 | -1 (0.74026) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.33829 HOMO: -6.86271 LUMO: 1.91296 factor:1 | -1 (0.45046) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.30035 HOMO: -6.50624 LUMO: 1.89119 factor:1 | -1 (0.48839) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76422 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-0.97547) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.93302 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.14427) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18410 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-0.39535) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74061 HOMO: -6.23413 LUMO: 1.91024 factor:1 | -1 (0.04814) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49031 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-0.70156) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36647 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.57772) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68800 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.89925) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73375 HOMO: -6.61509 LUMO: 2.31297 factor:1 | -1 (0.05499) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62779 HOMO: -6.45998 LUMO: 2.23405 factor:1 | -1 (0.16096) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.88137 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-0.09263) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24655 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.45780) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.82457 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.03583) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55197 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-0.76322) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83835 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.04961) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76843 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.97969) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.18401 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-1.39526) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89402 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.10528) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.14861 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-0.35987) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.03084 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.24210) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.12150 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-1.33276) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.28664 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.50210) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39912 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.61038) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38893 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (0.39982) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.94386 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (0.84489) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.29379 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.50504) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.62319 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (0.16555) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.98365 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (1.80509) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33615 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.54741) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68405 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.89531) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71654 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.92780) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49548 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.70673) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.60057 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-0.81182) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.60167 HOMO: -6.54434 LUMO: 2.20140 factor:1 | -1 (1.18707) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30573 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.51699) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.59365 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (1.19510) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38488 HOMO: -6.70761 LUMO: 2.71025 factor:1 | -1 (1.40386) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09523 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.30648) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95392 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.16517) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.20558 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (0.58317) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.20203 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-0.41329) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34522 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-0.55647) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73906 HOMO: -6.99061 LUMO: 2.13881 factor:1 | -1 (0.04969) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.60095 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.81221) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32301 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.53427) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69281 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.90407) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19814 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.40940) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.40414 HOMO: -6.78108 LUMO: 1.93745 factor:1 | -1 (0.38461) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44046 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.65171) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.34383 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.55509) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.19060 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.40186) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.53113 HOMO: -7.03414 LUMO: -0.69661 factor:1 | -1 (0.25761) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.32476 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (0.46398) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.06827 HOMO: -6.60692 LUMO: 2.12793 factor:1 | -1 (0.72048) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01449 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.22575) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.82366 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.03491) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57909 HOMO: -6.84094 LUMO: 1.66534 factor:1 | -1 (1.20965) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.23514 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (1.55361) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47269 HOMO: -6.60692 LUMO: 2.20684 factor:1 | -1 (1.31605) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.14792 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (1.64082) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.91426 HOMO: -6.31032 LUMO: 1.76330 factor:1 | -1 (1.87448) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34885 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (1.43989) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.97002 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (1.81873) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.10862 HOMO: -6.40556 LUMO: 2.02181 factor:1 | -1 (0.68012) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92878 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (0.85996) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53336 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.74461) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47140 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.68265) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51300 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.72426) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83293 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.04419) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.18760 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.39886) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.72884 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.94010) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69281 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-0.90407) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24383 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.45508) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61417 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.82543) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56182 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.77308) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.40931 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (0.37944) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43920 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-0.65046) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32971 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-0.54096) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.38865 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-0.59990) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.58934 HOMO: -6.72665 LUMO: 2.28848 factor:1 | -1 (0.19941) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.81505 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (1.97370) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15601 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (1.63274) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.31684 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (0.47190) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.04348 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (0.74527) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11738 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.32863) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36358 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.57484) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25898 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-0.47024) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.95533 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-0.16659) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11825 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.32950) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92440 HOMO: -6.26406 LUMO: 2.21773 factor:1 | -1 (0.86434) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.71588 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (1.07286) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12432 HOMO: -6.67767 LUMO: 2.34834 factor:1 | -1 (0.66442) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.79319 HOMO: -6.52801 LUMO: 2.10344 factor:1 | -1 (0.99556) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.56346 HOMO: -6.52801 LUMO: 2.24222 factor:1 | -1 (0.22528) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59445 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.80570) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47972 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.69098) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46821 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-0.67947) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.25349 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-0.46474) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.64441 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-0.85566) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53518 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.74644) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44671 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-0.65797) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26641 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.47767) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31583 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.52708) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52927 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.74053) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43237 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-0.64363) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28687 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (1.50188) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.05336 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (1.73538) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.02596 HOMO: -6.74570 LUMO: 2.20684 factor:1 | -1 (1.76278) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.77959 HOMO: -6.30216 LUMO: 2.15242 factor:1 | -1 (2.00915) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.89603 HOMO: -6.94979 LUMO: 2.43814 factor:1 | -1 (1.89272) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20433 HOMO: -6.97972 LUMO: 2.11432 factor:1 | -1 (1.58441) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.07092 HOMO: -6.17154 LUMO: 1.98099 factor:1 | -1 (1.71783) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.20140 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.41266) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.06317 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.27443) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26160 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.47285) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.87621 HOMO: -6.34297 LUMO: 1.92657 factor:1 | -1 (0.91253) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15430 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.36556) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43288 HOMO: -6.75114 LUMO: 1.98643 factor:1 | -1 (1.35586) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24520 HOMO: -6.69128 LUMO: 2.08711 factor:1 | -1 (1.54354) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51188 HOMO: -6.65318 LUMO: 2.15514 factor:1 | -1 (1.27687) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26869 HOMO: -6.67495 LUMO: 1.72248 factor:1 | -1 (1.52006) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50124 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (1.28751) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29979 HOMO: -6.61237 LUMO: 1.69799 factor:1 | -1 (1.48895) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.96006 HOMO: -6.57427 LUMO: 2.29936 factor:1 | -1 (1.82869) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32202 HOMO: -6.40012 LUMO: 2.35378 factor:1 | -1 (1.46672) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37212 HOMO: -6.90081 LUMO: 2.26671 factor:1 | -1 (1.41662) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35772 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (1.43102) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.13410 HOMO: -6.61509 LUMO: 2.26943 factor:1 | -1 (1.65464) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.96008 HOMO: -6.78924 LUMO: 2.09256 factor:1 | -1 (1.82866) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30159 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (1.48716) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15775 HOMO: -6.75931 LUMO: 1.98643 factor:1 | -1 (1.63100) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.97652 HOMO: -6.17971 LUMO: 2.09800 factor:1 | -1 (1.81222) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.73886 HOMO: -6.83006 LUMO: 1.91840 factor:1 | -1 (2.04989) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38521 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (1.40354) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20025 HOMO: -6.78924 LUMO: 2.42726 factor:1 | -1 (1.58849) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.51729 HOMO: -6.41372 LUMO: 1.93745 factor:1 | -1 (1.27145) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43275 HOMO: -6.85455 LUMO: 2.14970 factor:1 | -1 (1.35600) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.05132 HOMO: -6.38651 LUMO: 2.18507 factor:1 | -1 (1.73742) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29574 HOMO: -6.81373 LUMO: 2.00548 factor:1 | -1 (1.49301) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46749 HOMO: -6.64774 LUMO: 2.41365 factor:1 | -1 (1.32125) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22316 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (1.56558) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27424 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (1.51450) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.47291 HOMO: -6.81101 LUMO: 1.86670 factor:1 | -1 (1.31583) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34597 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (1.44277) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.89325 HOMO: -6.35930 LUMO: 1.78507 factor:1 | -1 (1.89549) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.09380 HOMO: -6.38651 LUMO: 2.04358 factor:1 | -1 (1.69494) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.85045 HOMO: -6.42189 LUMO: 1.99187 factor:1 | -1 (1.93829) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.11097 HOMO: -6.69400 LUMO: 1.61091 factor:1 | -1 (1.67777) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35465 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (1.43409) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.95591 HOMO: -6.90897 LUMO: 2.28576 factor:1 | -1 (0.83283) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.74014 HOMO: -6.75387 LUMO: 2.31297 factor:1 | -1 (0.04860) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.26024 HOMO: -7.05863 LUMO: 2.18780 factor:1 | -1 (0.52850) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.41763 HOMO: -6.56611 LUMO: 1.99187 factor:1 | -1 (0.37111) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46803 HOMO: -6.59060 LUMO: 1.86398 factor:1 | -1 (0.32071) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.49584 HOMO: -6.59060 LUMO: 1.59459 factor:1 | -1 (0.29290) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.32631 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.46243) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51570 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.72695) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67608 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.88734) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57121 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.78246) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.78362 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.99488) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.86058 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.07184) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11484 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.32610) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.94105 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.15230) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49817 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.70943) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47295 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.68420) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.04676 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.25802) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.05045 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-1.26171) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.27253 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.48379) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04256 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.25382) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44144 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.65269) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26766 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.47892) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.41890 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.63016) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.35528 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.56654) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67859 HOMO: -6.64774 LUMO: 2.13337 factor:1 | -1 (0.11015) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.45069 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (2.33806) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46514 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.67639) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.67230 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.88355) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71336 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.92462) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.54356 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.75482) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.53850 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.74976) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.66875 HOMO: -6.55794 LUMO: 2.06807 factor:1 | -1 (1.11999) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46587 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.67713) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15931 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.37056) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44979 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.66105) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24804 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.45930) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89304 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.10430) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.30131 HOMO: -6.85727 LUMO: 2.27759 factor:1 | -1 (1.48743) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41724 HOMO: -6.91713 LUMO: 2.28848 factor:1 | -1 (1.37151) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.15707 HOMO: -7.10217 LUMO: 2.14698 factor:1 | -1 (1.63168) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34961 HOMO: -6.78108 LUMO: 2.45447 factor:1 | -1 (1.43913) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.22189 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.43315) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23613 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.44738) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.94731 HOMO: -6.72665 LUMO: 2.25855 factor:1 | -1 (0.84143) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01408 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.22534) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.74342 HOMO: -6.17426 LUMO: 1.45853 factor:1 | -1 (1.04533) | -1 | -1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.05237 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.26362) | 1 | 1 |
| G: -5750.42305 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.89816 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.10942) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37231 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (1.41643) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.20733 HOMO: -7.19469 LUMO: 1.60819 factor:1 | -1 (1.58142) | 1 | 1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37326 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (1.41548) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22923 HOMO: -6.70489 LUMO: 0.74559 factor:1 | -1 (1.55951) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.12586 HOMO: -6.72393 LUMO: 0.88981 factor:1 | -1 (1.66289) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29258 HOMO: -4.54430 LUMO: -0.90614 factor:1 | -1 (1.49616) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28594 HOMO: -6.83006 LUMO: 0.47348 factor:1 | -1 (1.50280) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.17886 HOMO: -7.07496 LUMO: 0.50613 factor:1 | -1 (1.60988) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.83344 HOMO: -6.62053 LUMO: 0.74559 factor:1 | -1 (1.95530) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37745 HOMO: -6.79196 LUMO: 1.80139 factor:1 | -1 (1.41129) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.04150 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (1.74724) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.41913 HOMO: -6.74026 LUMO: 0.95784 factor:1 | -1 (0.36961) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.34250 HOMO: -7.34707 LUMO: 0.40001 factor:1 | -1 (0.44624) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38153 HOMO: -6.19875 LUMO: -0.88709 factor:1 | -1 (0.40722) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.13766 HOMO: -6.48719 LUMO: -0.14694 factor:1 | -1 (0.65109) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.03140 HOMO: -6.73482 LUMO: -0.01633 factor:1 | -1 (0.75735) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.61606 HOMO: -7.05591 LUMO: -0.20136 factor:1 | -1 (0.17268) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.38691 HOMO: -6.38651 LUMO: -2.07895 factor:1 | -1 (0.40183) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43918 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.65043) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.30538 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.51664) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26391 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.47517) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.90719 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.11844) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.73530 HOMO: -6.68040 LUMO: 0.21225 factor:1 | -1 (0.05344) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.83691 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.04816) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.50375 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-0.71501) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.95500 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.16625) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21139 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-0.42265) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.23194 HOMO: -6.75931 LUMO: -0.73471 factor:1 | -1 (0.55680) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11463 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.32588) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46384 HOMO: -6.34297 LUMO: 0.35375 factor:1 | -1 (0.32490) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33074 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.54200) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.37768 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.58894) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.16402 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.37527) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.57821 HOMO: -6.96884 LUMO: -0.31021 factor:1 | -1 (0.21053) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.29543 HOMO: -6.51713 LUMO: -0.59865 factor:1 | -1 (0.49332) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.97073 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.18199) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01830 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.22956) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.80493 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.01619) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.33568 HOMO: -6.79740 LUMO: -0.24762 factor:1 | -1 (1.45306) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31389 HOMO: -6.91986 LUMO: -0.14694 factor:1 | -1 (1.47486) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.99355 HOMO: -6.75114 LUMO: 0.18504 factor:1 | -1 (1.79519) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.10710 HOMO: -6.74842 LUMO: 0.69389 factor:1 | -1 (0.68165) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.95330 HOMO: -7.01782 LUMO: 0.56600 factor:1 | -1 (0.83544) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.01967 HOMO: -6.47359 LUMO: -0.56600 factor:1 | -1 (0.76908) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12699 HOMO: -6.63686 LUMO: -0.55783 factor:1 | -1 (0.66175) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.81077 HOMO: -4.13885 LUMO: -2.05446 factor:1 | -1 (0.97798) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.64784 HOMO: -6.34570 LUMO: 0.19864 factor:1 | -1 (0.14090) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46584 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.67710) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.06566 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.27692) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.45904 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.67030) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21640 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.42765) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55289 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.76415) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47444 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.68570) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.52919 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.74045) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44258 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.65384) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46484 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.67609) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.64733 HOMO: -6.37291 LUMO: -0.69117 factor:1 | -1 (0.14142) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36598 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.57724) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.31011 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.52137) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.23841 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-0.44967) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.51946 HOMO: -6.57155 LUMO: -0.34831 factor:1 | -1 (0.26928) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.49744 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.70869) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.03171 HOMO: -6.91713 LUMO: -0.69933 factor:1 | -1 (2.75703) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.88248 HOMO: -6.80557 LUMO: -0.65035 factor:1 | -1 (1.90627) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.09143 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (1.69731) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12012.94514 HOMO: -6.69128 LUMO: -0.16871 factor:1 | -1 (1.84360) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.12536 HOMO: -6.88448 LUMO: 0.13061 factor:1 | -1 (0.66339) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.19695 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (0.59179) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.97466 HOMO: -6.56067 LUMO: 0.17687 factor:1 | -1 (0.81408) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15983 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.37108) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.08899 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.30025) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.96973 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.18098) | -1 | -1 |
| G: -5750.42305 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.15792 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.36918) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.13268 HOMO: -6.51168 LUMO: -0.76464 factor:1 | -1 (3.19437) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12447.93757 HOMO: -7.14571 LUMO: -0.80274 factor:1 | -1 (3.38948) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.36406 HOMO: -6.66679 LUMO: -0.88709 factor:1 | -1 (2.96299) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.30765 HOMO: -6.76203 LUMO: -1.43948 factor:1 | -1 (3.01940) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.30076 HOMO: -6.57427 LUMO: -1.62996 factor:1 | -1 (3.02629) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.78438 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-1.45733) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.42813 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.10108) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.34614 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.01909) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.72903 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-1.40199) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.40149 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.07444) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.87805 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-0.55100) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.62117 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.29412) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.54756 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.22051) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.68156 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.35451) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.47842 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.15137) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.23569 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.90864) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.25863 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.93158) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.26633 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.93928) | 1 | 1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.33885 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.01180) | 1 | 1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.09264 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.76559) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.44827 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.12122) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.10685 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.77980) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.47235 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.14530) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.67135 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.34430) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.41412 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.08707) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.26040 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.93335) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12450.99502 HOMO: -6.80557 LUMO: -0.88165 factor:1 | -1 (0.33203) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.59377 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.26672) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.00897 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-0.68192) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.13093 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.80388) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.15199 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.82494) | 1 | 1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.52740 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.20035) | 1 | 1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.71555 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.38850) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.69835 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.37130) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.38530 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.05825) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.39583 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.06878) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.87128 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.54423) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.17188 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.84483) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.45749 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.13044) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.01993 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.69288) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.12845 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.80140) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.23466 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.90761) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.98238 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.65533) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.30949 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.98244) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.18266 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.85561) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.08451 HOMO: -6.91441 LUMO: -1.04492 factor:1 | -1 (0.24254) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.46745 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-1.14040) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.75748 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.43043) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.25333 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.92628) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.46816 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-1.14111) | -1 | -1 |
| G: -6186.96136 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.02853 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.70148) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.13268 HOMO: -6.48992 LUMO: 1.44765 factor:1 | -1 (2.84011) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12447.93757 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (3.03521) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.36406 HOMO: -6.62325 LUMO: 1.57826 factor:1 | -1 (2.60873) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.30765 HOMO: -6.19875 LUMO: 1.29798 factor:1 | -1 (2.66514) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12448.30076 HOMO: -6.74570 LUMO: 1.52112 factor:1 | -1 (2.67202) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.78438 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-1.81160) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.42813 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-1.45535) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.34614 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-1.37336) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.72903 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-1.75625) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.40149 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-1.42871) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.87805 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.90527) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.62117 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-1.64838) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.54756 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-1.57478) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.68156 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.70877) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.47842 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-1.50563) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.23569 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-1.26291) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.25863 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-1.28585) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.26633 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-1.29355) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.33885 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.36607) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.09264 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-1.11986) | -1 | -1 |
| G: -6186.60709 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.44827 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-1.47548) | -1 | -1 |
| G: -6186.60709 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.10685 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-1.13406) | 1 | 1 |
| G: -6186.60709 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.47235 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-1.49957) | -1 | -1 |
| G: -6186.60709 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.67135 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-1.69856) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.41412 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-1.44133) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.26040 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-1.28762) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12450.99502 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.02223) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.59377 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-1.62098) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.00897 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-1.03618) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.13093 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.15814) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.15199 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.17921) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.52740 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.55461) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.71555 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.74276) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.69835 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-0.72556) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.38530 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.41252) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.39583 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.42305) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.87128 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.89849) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.17188 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-1.19910) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.45749 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-1.48471) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.01993 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.04715) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.12845 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.15567) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.23466 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.26187) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.98238 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-1.00960) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.30949 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-1.33670) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.18266 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-1.20987) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.08451 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.11173) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.46745 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-1.49467) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12451.75748 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.78469) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.25333 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-1.28054) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.46816 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.49537) | -1 | -1 |
| G: -6186.60709 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12452.02853 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.05575) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.32376) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.82314) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-2.71586) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-2.15607) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.78262) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.73653) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.47507) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.56063) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-2.18358) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-1.49113) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-2.04698) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-2.07726) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.76902) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-2.15762) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-1.62335) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-1.66599) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-1.67328) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.72817) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.79370) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.78208) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.69220) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.79732) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.78238) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.53625) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-2.75932) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.95797) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.62213) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-2.03506) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-2.09424) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.45619) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.62085) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.57023) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.61574) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.64913) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.74771) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.94102) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.95022) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.89074) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.05020) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.85678) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.46196) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.59581) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-1.37377) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.74581) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.72464) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.89615) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.77376) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.83109) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.76499) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.47216) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-1.68134) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.62185) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.84529) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.33243) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.45799) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.41975) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.49254) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-1.25975) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.27279) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-1.54887) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-2.77513) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-2.00815) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-1.79100) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-2.14657) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.77732) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-2.29259) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.74683) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.83920) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.68516) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.46472) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.61087) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.76129) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.33788) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-1.39262) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.56593) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-1.72898) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-1.48014) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.42806) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.41742) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-2.63423) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.73124) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.38980) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-2.00213) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-2.11465) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.33959) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.35850) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.73901) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.84305) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.74572) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-2.28401) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-0.96590) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.49048) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.31926) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.08323) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.03387) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.00328) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.19665) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.04731) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-0.87052) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.91950) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.62074) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.57459) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-1.43755) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.72732) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.56931) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.60868) | 1 | 1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.71302) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-1.54003) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.68683) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.53401) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.49834) | -1 | -1 |
| G: -6289.55979 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.76561) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.65176) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.76357) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.57701) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.69258) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.49459) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.42231) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-0.80287) | 1 | 1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.51565) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.44340) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.46392) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-1.55807) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.67358) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-1.78624) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.95153) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.39532) | 1 | 1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.06165) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.34879) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.10037) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.46688) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.54348) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.53704) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.51475) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.11763) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.08231) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.34068) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.22163) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.18087) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.80774) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-1.00252) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.98892) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.93025) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.55873) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-1.06783) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.69569) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-1.43355) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.96959) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.93108) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-2.49803) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-2.32997) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-2.01046) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.61698) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.93372) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.88578) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-2.13808) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-2.47199) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-2.47128) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.62892) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-1.98948) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-2.68144) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-2.53183) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.72893) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.96246) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-2.64549) | -1 | -1 |
| G: -6289.55979 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-2.51583) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-2.18374) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.92085) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.63146) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.49002) | 1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.35456) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.51801) | -1 | -1 |
| G: -6289.55979 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.56732) | 1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.76060) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.45409) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.87308) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.73136) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.65139) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.82761) | -1 | -1 |
| G: -6289.55979 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.82385) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.52779) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-2.12132) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-2.56326) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.62978) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-1.96466) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.30770) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.62950) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-2.20020) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.85021) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.59173) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-1.50645) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-1.65668) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-1.28699) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-1.63285) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.92997) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-1.50335) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.35201) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.53859) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.07146) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.64083) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-1.40661) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-2.01552) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.55663) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.26313) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.94306) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.87116) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-2.03051) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-1.66882) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-1.50231) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.44482) | -1 | -1 |
| G: -6289.55979 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.79162) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.49995) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.85693) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.90423) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.04972) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.73554) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.58670) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.50673) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.68638) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.39492) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.67430) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.47630) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.04722) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.42079) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.27561) | 1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.62076) | 1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.96044) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.40438) | 1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.26068) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.49325) | 1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.54914) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.27668) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.18206) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.97036) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.12527) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.42461) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.60880) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.75691) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.91988) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.79476) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.40975) | -1 | -1 |
| G: -6289.55979 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.48844) | 1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.82274) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.46306) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.70175) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.36817) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.85316) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.53849) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.70722) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.70388) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.37680) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.27595) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.46406) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.50142) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.60453) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.51470) | 1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.32569) | 1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.82143) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.74224) | 1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.87506) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.74186) | 1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.48771) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.59830) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.63824) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.27328) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.33952) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.50055) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.54023) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.63593) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.61832) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.75286) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.49783) | -1 | -1 |
| G: -6289.55979 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.53547) | 1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.17621) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.28157) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.37505) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.42403) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.06239) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.06943) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.43439) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.23295) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.77873) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.87584) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.65053) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.62971) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.91174) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.48007) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.34657) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.67837) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.16497) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.53317) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.54030) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.43725) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.78629) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.47309) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.68891) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.69302) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.37786) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.78761) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.57451) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.36501) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.61982) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.46681) | -1 | -1 |
| G: -6289.55979 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.94499) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.48002) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.61279) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.59520) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.30325) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.34420) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.56104) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.34760) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.95419) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.18419) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.35905) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.13196) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.26459) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.87628) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.04143) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.53671) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.58920) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.36106) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.41407) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.50759) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.34688) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.36566) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.16786) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.77576) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.54672) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.75026) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.32176) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.50449) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.09868) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.35954) | -1 | -1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.52087) | 1 | 1 |
| G: -6289.55979 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.37407) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.21447) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.52521) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.36180) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.36061) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.49070) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.53440) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.24678) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.25829) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.49859) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.31407) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.08904) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.43454) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.32425) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.76909) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.61542) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.55012) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.25029) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.40273) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.37742) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.98387) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.30250) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.83478) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.22459) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.38310) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.10437) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.47064) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.26059) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.31208) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.73830) | -1 | -1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.60262) | 1 | 1 |
| G: -6289.55979 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.79006) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.60613) | 1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-0.44199) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-0.77678) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-1.05439) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.00475) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.88393) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-0.51021) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-1.04119) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-0.77806) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-0.92132) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-0.82508) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-0.92949) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.94671) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-0.76687) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-0.60796) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.77555) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-0.75852) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-0.44594) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-0.78997) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-0.82339) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.44781) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.48770) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.68947) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-1.66980) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-1.59878) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.53627) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.87515) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.00617) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-0.86622) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.11939) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.39818) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.31932) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.38160) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.44275) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.32930) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.06309) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.56982) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.50430) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.35943) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.16495) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.18040) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.41061) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.44258) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.18130) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.01675) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.36822) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.42593) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.70494) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.64257) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.46793) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.28909) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.21494) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.84747) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.53302) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-0.69139) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-0.77457) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.58200) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-0.41840) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-0.66559) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-0.56624) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.69800) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.49359) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-0.34869) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-0.63275) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.31864) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.35502) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-1.28000) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-0.92706) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.34778) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.14984) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.82508) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.59811) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.67743) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.32822) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.74992) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.42246) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.27070) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.54608) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.52004) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.70510) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.82086) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.90698) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.65979) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.62124) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.49699) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.61609) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-0.63000) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.37168) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.68959) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-0.34289) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.44586) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.26077) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.07902) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.58129) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.24958) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.84026) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.73231) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.22427) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.25474) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-1.11591) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.43565) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.48491) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.33617) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.04645) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.14781) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.15647) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.51481) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-0.24999) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.92622) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.79974) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-0.70684) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.89800) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.61773) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.71884) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-1.47341) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-1.59176) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-1.63184) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-1.38043) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.42952) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.80853) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.87487) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-0.70815) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-0.59656) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-0.50292) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-0.42657) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-0.46447) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.19045) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.55759) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-1.42852) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.62403) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-1.16375) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.59312) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-1.43807) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.88026) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.62077) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.75697) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.44763) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.25290) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.47277) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.67990) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-0.83076) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-0.52243) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-0.63383) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-0.69713) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.27056) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-0.27342) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-0.00495) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-0.41380) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.62554) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-0.61797) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-1.59902) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-1.66251) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.41682) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-1.45184) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.28250) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.31553) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.27009) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-1.45592) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.35736) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-1.09199) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.43317) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.33181) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.35336) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-1.18310) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.39807) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-1.43423) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.58917) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-1.42386) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-1.24375) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-1.17542) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.46746) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.47722) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-1.51276) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.30672) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-1.47663) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-1.10437) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-1.06666) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-1.39521) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-1.24685) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-0.52787) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-0.64056) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.66858) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.78284) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.40398) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.46118) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.51157) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.70018) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-0.59400) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-0.56374) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-0.41285) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-1.52781) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.54378) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-1.29012) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-1.61976) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.38310) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-1.23170) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-1.04835) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.45494) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-1.24525) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-1.41807) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-1.37317) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-1.18002) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.08217) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.46952) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.32626) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.02494) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.98051) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.86783) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.53928) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-1.26998) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-1.13471) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.93090) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-1.31499) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-1.13768) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-1.27605) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-1.49271) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-1.04530) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.98160) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-1.06584) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-1.43137) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-1.23066) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-1.30242) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-1.21412) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-1.43807) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.93509) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-0.80812) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.90940) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.54450) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-1.19080) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-0.98723) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.98285) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.90127) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-0.71471) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-1.18633) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-1.88009) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-2.65719) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.53434) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.67611) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.88115) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.47165) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.97095) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-2.47874) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-2.19645) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-2.65466) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.49625) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.31268) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.13017) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-2.59605) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.81413) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-2.74166) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.43725) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-2.20709) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-1.96224) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.74817) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.60075) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.46967) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-2.01438) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-1.47260) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.86485) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.41671) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-1.36062) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-1.47050) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.39241) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.53380) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.31956) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-1.18710) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-1.25602) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.96562) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.70819) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.89900) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.70131) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.92793) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-2.50791) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.73426) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-2.20472) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-2.29155) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-1.57151) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-2.13664) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.41820) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.49260) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.69603) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-1.54014) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-1.31164) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-1.32715) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.67906) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.45832) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.37661) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.63639) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.58660) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.18841) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.46330) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.39304) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-0.42442) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.26210) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.62110) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.39914) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.79239) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-2.58285) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-2.33351) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.68025) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-0.24158) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-0.47174) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.94229) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.27238) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-2.07835) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-1.98170) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.76479) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.04606) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-1.35371) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.48204) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-1.44656) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.42852) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.34416) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.63946) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.66267) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.43965) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.48313) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-1.18002) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.30213) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.15652) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-0.17442) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (0.08555) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.35911) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-2.07413) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-1.81429) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-2.13160) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-1.40299) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-1.12974) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.97428) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-1.16731) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-1.31967) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.30147) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-1.00337) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-1.11959) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.86856) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-1.30928) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.46395) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.65960) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.59465) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-0.56088) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.26692) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-0.40637) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.62948) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.85866) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.82987) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-0.55473) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.63190) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-0.30575) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-0.40964) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-0.27973) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.11954) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.41018) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.64867) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.70227) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.42782) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.64736) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.54494) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.74478) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.24503) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-1.41042) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-1.11782) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-1.18506) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.09893) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.15632) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.64437) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.38831) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.20746) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-0.02950) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.32852) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-0.45884) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-0.41650) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.37225) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.13222) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.32866) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.23209) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.07684) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.57827) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.24419) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-0.57411) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.41059) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.20460) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (0.09589) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.39979) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.58684) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-0.52687) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-0.33704) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-0.33960) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (0.01589) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.15554) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.17883) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.77019 LUMO: 0.92247 factor:1 | -1 (0.09312) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.44425) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.74282) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.50945) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.65522) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.74078) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.80314) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.51378) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.46651) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.71585) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.41481) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.65930) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.70390) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-0.49435) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.35775) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.43965) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.55710) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.60243) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.40180) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.21453) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.74570 LUMO: -0.75103 factor:1 | -1 (0.06123) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.46670) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.44476) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-1.46863) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-1.45314) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.03071) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.25624) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-1.16682) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.23828) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.67648) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.42640) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.46063) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.28047) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.23549) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.17568) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.00982) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.42561) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.39892) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-1.28196) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.12938) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-1.56914) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-0.91811) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.95760) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.05422) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-1.08203) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.21463) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.20835) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.11575) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.05969) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.83446) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-0.95085) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.00603) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.29806) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.07757) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.12617) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.37349) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-2.49561) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.87076) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-2.65189) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-1.66686) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-1.68458) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-2.51096) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-2.47278) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-2.09084) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-2.47210) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-2.27528) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.48694) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.05798) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-2.23528) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-1.34318) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.12299) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.68664) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-1.40729) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.50996) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-1.55595) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-1.43026) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.87378) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.68139) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-1.71924) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.69026) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.31407) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.47465) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-0.32425) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.51976) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-1.39594) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-2.11275) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-2.04624) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.41064) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.88850) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.24337) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.43845) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-1.36027) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.33050) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.37426) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-1.01033) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-1.14873) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.11469) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.94083) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-1.33534) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-0.46006) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-0.52779) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-0.32509) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-0.53149) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-0.38017) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.52276) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.29693) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-0.50270) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-0.39628) | 1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-0.33954) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-0.53770) | 1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-0.36567) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.33767) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.38624) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.30874) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.44316) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.38727) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.59016) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.48477) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.36373) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.04980) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.28311) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-0.47778) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-0.27094) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-0.48499) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-0.40071) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-0.30860) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-0.51212) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-0.58094) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.04116) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-1.12429) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-0.97564) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-1.07610) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-1.16182) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-1.29796) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-1.43788) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-1.04171) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-1.53274) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-2.46130) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-2.24246) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-2.49787) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.57636) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-2.09354) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.48482) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-2.27980) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-2.33936) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.31581) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-2.12899) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.53151) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.35439) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-1.26274) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-1.41551) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.48384) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.33496) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.04391) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.54210) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-0.45565) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-0.47179) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-0.42779) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-0.05687) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-0.24033) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-0.32507) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.00873) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-0.19228) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.34909) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-0.25132) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.69777) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.43031) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-2.46965) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-2.38132) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.25305) | 1 | 1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-1.26824) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.27767 LUMO: -0.52790 factor:1 | -1 (0.04757) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-0.16607) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-0.32142) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-1.90896) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.87718) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.07852) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-1.76635) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-0.95104) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-0.97713) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-1.95587) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-1.17322) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.19442) | -1 | -1 |
| G: -6289.55979 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-1.30468) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (0.96443) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (0.46504) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-1.42767) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.86788) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.49443) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (0.55166) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-0.18689) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-0.27244) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.89539) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.20294) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.75879) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.78908) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.29671 LUMO: -0.89525 factor:1 | -1 (0.51917) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.86943) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.33516) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.37780) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.38510) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.43998) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -6.62325 LUMO: 0.31293 factor:1 | -1 (0.49449) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.59604 LUMO: 0.19592 factor:1 | -1 (0.50610) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.43277 LUMO: -0.27756 factor:1 | -1 (0.59598) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.54978 LUMO: -0.46531 factor:1 | -1 (0.49087) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.65046 LUMO: -0.15783 factor:1 | -1 (0.50581) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -7.28721 LUMO: 0.23946 factor:1 | -1 (0.75193) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.47113) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.66978) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.53345 LUMO: -0.84627 factor:1 | -1 (0.66605) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.74687) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-0.80606) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.16800) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-0.33266) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-0.28205) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.43549 LUMO: 0.14150 factor:1 | -1 (0.67245) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.63906) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (0.54047) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.33753 LUMO: -0.02993 factor:1 | -1 (0.34716) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.49808 LUMO: -0.83811 factor:1 | -1 (0.33797) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (0.39745) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (0.23799) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (0.43141) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-0.17377) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-0.30762) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-0.08558) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.54238) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.56355) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (0.39203) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.51443) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.45710) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (0.52319) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-0.18398) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-0.39315) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-0.33367) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (0.44289) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-0.04425) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-0.16980) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.13157) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.20436) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (0.02844) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.29944 LUMO: 1.40955 factor:1 | -1 (0.01540) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.26069) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.48694) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.71996) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.50281) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.85838) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.60148 LUMO: -1.04764 factor:1 | -1 (0.51087) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.00440) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-0.45865) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.54434 LUMO: 0.11157 factor:1 | -1 (0.44899) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.53617 LUMO: 0.32926 factor:1 | -1 (0.60303) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.62597 LUMO: -0.60137 factor:1 | -1 (0.82347) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.60965 LUMO: -0.75376 factor:1 | -1 (0.67732) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.29399 LUMO: 0.06803 factor:1 | -1 (0.52689) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-0.04969) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.10444) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.27775) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.44080) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-0.19195) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (0.86012) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (0.87076) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-1.34604) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.44306) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.36474 LUMO: 1.61091 factor:1 | -1 (0.89838) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.71395) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-0.82646) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.05140) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-0.07031) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.54918) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.55487) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-0.45753) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.99583) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (0.32229) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-0.20229) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-0.03108) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.46815 LUMO: 1.59459 factor:1 | -1 (0.20496) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.31304 LUMO: 1.36873 factor:1 | -1 (0.25432) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.22597 LUMO: 1.54833 factor:1 | -1 (0.28490) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -5.63004 LUMO: 1.96466 factor:1 | -1 (0.09154) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (0.24088) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.78924 LUMO: 2.10888 factor:1 | -1 (0.41767) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.13345 LUMO: 2.07351 factor:1 | -1 (0.36869) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-0.33255) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-0.28640) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.14936) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-0.43914) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.28112) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-0.32050) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.57517) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.25184) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.39865) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.24583) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.21015) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.47742) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.36357) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.47538) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.28882) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-0.40439) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.20640) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.13412) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (0.48532) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.22746) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.15521) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.17573) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-0.26988) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.38539) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.49805) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.33666) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-0.10713) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.91713 LUMO: 1.87486 factor:1 | -1 (0.22653) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.06060) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.18781) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.17870) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-0.25530) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.24885) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.22656) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -6.66135 LUMO: -0.75648 factor:1 | -1 (0.17056) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -7.56749 LUMO: 0.22585 factor:1 | -1 (0.20588) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.05249) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.31032 LUMO: -0.34286 factor:1 | -1 (0.06656) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.10732) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.61781 LUMO: 1.98915 factor:1 | -1 (0.48044) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (0.28567) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.44094 LUMO: 1.80956 factor:1 | -1 (0.29927) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.35794) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.72946) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.22036) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.59250) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-0.14536) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-0.68140) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.64290) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-1.20985) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.04179) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-0.72227) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.32880) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-0.64554) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.59759) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-0.84989) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.18380) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.18310) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.34073) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-0.70129) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.39325) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.24364) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-0.44074) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-0.67427) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.35730) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.22764) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.89555) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-0.63266) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.34327) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.49264 LUMO: -0.74559 factor:1 | -1 (0.79816) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.67223 LUMO: -0.55239 factor:1 | -1 (0.93362) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.22983) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-0.27913) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-0.47242) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-0.16591) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.41511) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.57155 LUMO: -0.67484 factor:1 | -1 (0.55683) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.53345 LUMO: -0.78913 factor:1 | -1 (0.63680) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -7.07768 LUMO: 0.28844 factor:1 | -1 (0.46058) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.75114 LUMO: 0.18776 factor:1 | -1 (0.46434) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.77019 LUMO: -0.12245 factor:1 | -1 (0.76039) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-0.83313) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.27507) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.65841) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-0.67648) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-0.01951) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.34131) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.91202) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.56202) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.30354) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.21826) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-0.36850) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.51985 LUMO: -0.68028 factor:1 | -1 (0.00120) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-0.34466) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.64178) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.21516) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.93618) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.74959) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.10761 LUMO: 0.28028 factor:1 | -1 (1.21673) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.64736) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-0.11842) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-0.72733) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.26844) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (0.02506) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-0.65487) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-0.58298) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.74233) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-0.38063) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-0.21413) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.15663) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.50344) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.21176) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.56875) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.61604) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.76154) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-0.44736) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -5.91303 LUMO: 1.90480 factor:1 | -1 (0.70148) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (0.78146) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (0.60181) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.89327) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (0.61389) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.18811) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.75903) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.13260) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.98742) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-0.33258) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.67226) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.11619) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.29127 LUMO: 1.87486 factor:1 | -1 (0.02751) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.20507) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.26096) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.01151) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.10612) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.63414 LUMO: 1.62452 factor:1 | -1 (0.31783) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.16291) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (0.86358) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.20964 LUMO: 1.84221 factor:1 | -1 (0.67939) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.53128) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.44094 LUMO: 2.05446 factor:1 | -1 (0.36831) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.61509 LUMO: 2.16058 factor:1 | -1 (0.49342) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.65591 LUMO: 1.69527 factor:1 | -1 (0.87844) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.79974) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.68312 LUMO: 2.38100 factor:1 | -1 (0.46545) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.51168 LUMO: 2.14698 factor:1 | -1 (0.82513) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.04637 LUMO: 1.48302 factor:1 | -1 (0.58643) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.81645 LUMO: -0.74287 factor:1 | -1 (0.92002) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.96884 LUMO: -0.97961 factor:1 | -1 (0.43503) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.45998 LUMO: 0.09796 factor:1 | -1 (0.74970) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.44638 LUMO: 0.09524 factor:1 | -1 (0.58096) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.16338 LUMO: -0.54151 factor:1 | -1 (0.58431) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.35930 LUMO: -0.47892 factor:1 | -1 (0.91139) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.65318 LUMO: -0.00272 factor:1 | -1 (1.01224) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.82412) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.78676) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.60148 LUMO: -0.77552 factor:1 | -1 (0.68366) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.77348) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.96249) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (0.46676) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.54594) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (0.41312) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (0.54632) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.80048) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.68989) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.86543 LUMO: 1.98643 factor:1 | -1 (0.64994) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.69944 LUMO: 1.65173 factor:1 | -1 (1.01490) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.77836 LUMO: 2.16331 factor:1 | -1 (0.94867) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.42189 LUMO: 2.36467 factor:1 | -1 (0.78763) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -7.00965 LUMO: 2.04358 factor:1 | -1 (0.74796) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.36746 LUMO: 2.13881 factor:1 | -1 (0.65226) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.37835 LUMO: 1.89935 factor:1 | -1 (0.66986) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -7.03959 LUMO: 1.27349 factor:1 | -1 (0.53533) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.67495 LUMO: -0.89253 factor:1 | -1 (0.79035) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.71849 LUMO: -0.97961 factor:1 | -1 (0.75272) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.47903 LUMO: 0.01633 factor:1 | -1 (0.11197) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.38379 LUMO: 0.01088 factor:1 | -1 (0.00661) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.08686) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-0.13584) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.16610 LUMO: 2.15514 factor:1 | -1 (0.22580) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.35114 LUMO: 1.98643 factor:1 | -1 (0.21875) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-0.14621) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.89809 LUMO: 2.20684 factor:1 | -1 (0.05524) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.49054) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.58766) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-1.36234) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-1.34152) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.62355) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.19189) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.05839) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.39018) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.87678) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.24498) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.25211) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-0.14906) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-0.49810) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-0.18490) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.59928) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.59517) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.91033) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (0.50058) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (0.71367) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.32665 LUMO: 2.28031 factor:1 | -1 (0.92317) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -5.98378 LUMO: 2.16331 factor:1 | -1 (0.66837) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.08991 LUMO: 2.30208 factor:1 | -1 (0.82138) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.65680) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.19183) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.32460) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.30702) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.01507) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -7.21646 LUMO: 1.71976 factor:1 | -1 (0.94399) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -6.94162 LUMO: 2.21773 factor:1 | -1 (0.72714) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.34842 LUMO: 2.04358 factor:1 | -1 (0.94059) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.66600) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.34842 LUMO: 1.88303 factor:1 | -1 (0.10400) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.07086) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-0.84377) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.30216 LUMO: 1.41771 factor:1 | -1 (0.02359) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-0.58809) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.53617 LUMO: 1.72792 factor:1 | -1 (0.24675) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-0.24852) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.30101) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.07287) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-0.12588) | 1 | 1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-0.21941) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.05869) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.07747) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.12033) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-0.48757) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-0.25854) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.46208) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.03357) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.21630) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.81049) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.07135) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.23268) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.08588) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (0.07372) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.04637 LUMO: 2.23950 factor:1 | -1 (0.76298) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.44366 LUMO: 2.24766 factor:1 | -1 (0.92638) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (0.92758) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (0.79748) | -1 | -1 |
| G: -6290.84798 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.54434 LUMO: 1.99187 factor:1 | -1 (0.75378) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -6.17698 LUMO: -0.65852 factor:1 | -1 (1.04141) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (1.02990) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.55250 LUMO: -0.86804 factor:1 | -1 (0.78959) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (0.97411) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (1.19915) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.85365) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (0.96394) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-0.48091) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-1.32724) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.26194) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (1.03790) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (0.88546) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (0.91077) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.69569) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.01431) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-0.54660) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (0.06359) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.09491) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.81618) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-0.18245) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-0.97240) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-0.02389) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.54989) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (0.68556) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.81645 LUMO: -0.07347 factor:1 | -1 (0.49813) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (0.68205) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.71033 LUMO: -0.26395 factor:1 | -1 (0.84619) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.70489 LUMO: -0.09252 factor:1 | -1 (0.51141) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -6.23685 LUMO: 0.39729 factor:1 | -1 (0.23380) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -6.69400 LUMO: -0.05442 factor:1 | -1 (0.28343) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.36202 LUMO: 0.09796 factor:1 | -1 (0.40425) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.54978 LUMO: 0.15510 factor:1 | -1 (0.77797) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -6.77836 LUMO: 0.25851 factor:1 | -1 (0.24700) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -5.70623 LUMO: 0.73471 factor:1 | -1 (0.51013) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -5.58378 LUMO: 0.89253 factor:1 | -1 (0.36686) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -5.68718 LUMO: 0.87893 factor:1 | -1 (0.46311) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.35870) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (0.34148) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -4.45450 LUMO: 1.82044 factor:1 | -1 (0.52132) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -4.64226 LUMO: 1.70615 factor:1 | -1 (0.68023) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.51264) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -4.85723 LUMO: 0.93607 factor:1 | -1 (0.52967) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -4.72934 LUMO: 1.00410 factor:1 | -1 (0.84225) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -4.56335 LUMO: 1.56738 factor:1 | -1 (0.49821) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -5.48854 LUMO: 0.33198 factor:1 | -1 (0.46480) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.15962) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.19951) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-0.40129) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-0.38161) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-0.31059) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.24809) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.41304) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (0.28202) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -4.62321 LUMO: 1.82861 factor:1 | -1 (0.42197) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -5.83684 LUMO: 0.82178 factor:1 | -1 (0.16879) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-0.10999) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-0.03113) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-0.09342) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-0.15456) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.04112) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (0.22509) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-0.28164) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.21611) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.07124) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (0.12324) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -5.09669 LUMO: 0.72382 factor:1 | -1 (0.10778) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.12242) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.15440) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.10689) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.27143) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.08003) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.13774) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -5.98650 LUMO: 0.76736 factor:1 | -1 (0.58325) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -4.74839 LUMO: 1.88847 factor:1 | -1 (0.64562) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (0.82026) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (0.99909) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -5.09397 LUMO: 0.98505 factor:1 | -1 (1.07324) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.44072) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -5.04227 LUMO: 1.49935 factor:1 | -1 (0.75517) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -5.22731 LUMO: 0.88437 factor:1 | -1 (0.59680) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -4.95519 LUMO: 1.25717 factor:1 | -1 (0.51361) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -4.61233 LUMO: 1.27621 factor:1 | -1 (0.70619) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (0.86978) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.62260) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -4.97696 LUMO: 1.00138 factor:1 | -1 (0.72195) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (0.59019) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.79460) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (0.93950) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -5.87766 LUMO: 0.42994 factor:1 | -1 (0.65544) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.03045) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-0.06683) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.43821 LUMO: 0.15238 factor:1 | -1 (0.00819) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (0.36112) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.05959) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.49264 LUMO: 0.19592 factor:1 | -1 (0.13834) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -5.83956 LUMO: 0.12517 factor:1 | -1 (0.46311) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.50896 LUMO: 0.19048 factor:1 | -1 (0.69008) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.61076) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (0.95996) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (0.53827) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.86573) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (1.01749) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -5.74160 LUMO: 0.14694 factor:1 | -1 (0.74211) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -4.78376 LUMO: 0.92791 factor:1 | -1 (0.76815) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.58309) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -4.99329 LUMO: 0.85988 factor:1 | -1 (0.46733) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -4.93887 LUMO: 1.33608 factor:1 | -1 (0.38120) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.62839) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (0.66695) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.79120) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (0.67209) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (0.65819) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (0.91651) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -4.92254 LUMO: 0.93879 factor:1 | -1 (0.59860) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (0.94530) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -4.97696 LUMO: 0.89798 factor:1 | -1 (0.84233) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -5.00690 LUMO: 1.14288 factor:1 | -1 (1.02742) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (1.20917) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (0.70690) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -5.22459 LUMO: 0.99049 factor:1 | -1 (1.03860) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (0.44793) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.55587) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.06392) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (0.03344) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -7.64640 LUMO: -2.45175 factor:1 | -1 (0.17228) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.14746) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.80328) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (0.95202) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (1.24174) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (1.14037) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (1.44465) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (1.80300) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (1.03820) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -8.50356 LUMO: -1.79595 factor:1 | -1 (0.36197) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -7.79334 LUMO: -2.33746 factor:1 | -1 (0.48844) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -7.24367 LUMO: -0.85172 factor:1 | -1 (0.58134) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.39018) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.67046) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.54978 LUMO: 0.34831 factor:1 | -1 (0.56934) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.18523) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.30357) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.34365) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-0.09225) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.14134) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.86543 LUMO: 0.93879 factor:1 | -1 (0.47966) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -7.09673 LUMO: -0.69661 factor:1 | -1 (0.41331) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -7.74708 LUMO: 0.01088 factor:1 | -1 (0.58004) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.80557 LUMO: 0.46531 factor:1 | -1 (0.69163) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -7.29265 LUMO: 1.31975 factor:1 | -1 (0.78527) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.93618 LUMO: 0.29388 factor:1 | -1 (0.86162) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.53073 LUMO: 0.71022 factor:1 | -1 (0.82372) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.41917 LUMO: -1.24084 factor:1 | -1 (1.09773) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -6.67495 LUMO: -1.09118 factor:1 | -1 (0.73060) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.14033) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.33584) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -7.12666 LUMO: -0.67484 factor:1 | -1 (0.12444) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.30493) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.14988) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -7.36340 LUMO: -0.68301 factor:1 | -1 (0.40793) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.66741) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -7.81511 LUMO: -0.06531 factor:1 | -1 (0.53122) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.84056) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (1.03528) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -7.44776 LUMO: -1.00954 factor:1 | -1 (0.81542) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -7.47769 LUMO: -1.02859 factor:1 | -1 (0.60828) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.75659 LUMO: 0.39457 factor:1 | -1 (0.45742) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (0.76576) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -7.64096 LUMO: -1.43948 factor:1 | -1 (0.65435) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (0.59106) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (1.01762) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -7.03414 LUMO: 0.20409 factor:1 | -1 (1.01477) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -7.22734 LUMO: 0.31293 factor:1 | -1 (1.28323) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.93618 LUMO: 0.56055 factor:1 | -1 (0.87438) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.94707 LUMO: -0.88709 factor:1 | -1 (0.66265) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.86543 LUMO: -0.83267 factor:1 | -1 (0.67022) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.31084) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.37432) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.12863) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.16365) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.93074 LUMO: -0.81634 factor:1 | -1 (0.00569) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.02735) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -7.07224 LUMO: -0.68028 factor:1 | -1 (0.01810) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.16773) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-0.06917) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -5.94569 LUMO: -0.72110 factor:1 | -1 (0.19619) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-0.14498) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-0.04362) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-0.06517) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (0.10509) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-0.10988) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-0.14604) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-0.30099) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.13568) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.98244 LUMO: -1.82044 factor:1 | -1 (0.04444) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.37563 LUMO: -1.67622 factor:1 | -1 (0.11276) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-0.17927) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-0.18904) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-0.22458) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.01853) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-0.18844) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (0.18381) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.22153) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-0.10702) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (0.04133) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.76031) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (0.64763) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (0.61960) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.50534) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.88421) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (0.82701) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.67495 LUMO: 0.21769 factor:1 | -1 (0.77661) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.84911 LUMO: 0.38368 factor:1 | -1 (0.58801) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (0.69419) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (0.72445) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.81917 LUMO: 1.30887 factor:1 | -1 (0.87534) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.23962) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.25560) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.00193) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.33157) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.09491) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (0.05649) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.23984) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.16675) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.04294) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.12988) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-0.08498) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (0.10817) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (0.20602) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.18134) | 1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-0.03807) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.52801 LUMO: 0.98233 factor:1 | -1 (0.26324) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.76475 LUMO: 0.53334 factor:1 | -1 (0.30768) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (0.42036) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.57971 LUMO: 0.12789 factor:1 | -1 (0.74891) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.99333 LUMO: 0.51430 factor:1 | -1 (0.01820) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (0.15347) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.16066 LUMO: 1.77146 factor:1 | -1 (0.35729) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.02680) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (0.15051) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.60420 LUMO: 1.33880 factor:1 | -1 (0.01214) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.20452) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.80013 LUMO: 1.34696 factor:1 | -1 (0.24289) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (0.30659) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.22234) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-0.14319) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (0.05752) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-0.01423) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.07407) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-0.14988) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.35309) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (0.48006) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (0.37878) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -7.78518 LUMO: -2.36467 factor:1 | -1 (0.74369) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -7.96477 LUMO: -2.75651 factor:1 | -1 (0.09739) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -7.60286 LUMO: -2.35106 factor:1 | -1 (0.30096) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -7.38245 LUMO: -1.21635 factor:1 | -1 (0.30534) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (0.38692) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -8.07362 LUMO: -0.28028 factor:1 | -1 (0.57348) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.10185) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-0.59190) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-1.36900) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-0.24615) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.38793) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.59296) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.18346) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.68276) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-1.19055) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.90826) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.36647) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.20806) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.02449) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -7.74164 LUMO: -2.36195 factor:1 | -1 (0.15802) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.30786) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.52594) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-1.45347) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-0.14906) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.91890) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.67405) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.45998) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -7.36068 LUMO: 0.05714 factor:1 | -1 (0.68744) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.81852) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-0.72619) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-0.18441) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.57666) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-0.12852) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.07244) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.18232) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.10422) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-0.24561) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-0.03137) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -7.79878 LUMO: 0.30477 factor:1 | -1 (0.10109) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -7.87498 LUMO: 0.61770 factor:1 | -1 (0.03216) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.32256) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.42001) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-0.61081) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.41312) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.63974) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-1.21972) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-0.44608) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-0.91653) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.00337) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-0.28332) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-0.84845) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.13002) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.20441) | 1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-0.40784) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.25195) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.02346) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.03897) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -7.36068 LUMO: -1.14560 factor:1 | -1 (0.60913) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.96339 LUMO: 0.26939 factor:1 | -1 (0.82987) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.53617 LUMO: 0.22313 factor:1 | -1 (0.91158) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -7.33619 LUMO: -1.02587 factor:1 | -1 (0.65179) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (0.70159) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (1.09978) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.82489) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -7.43415 LUMO: 0.10612 factor:1 | -1 (0.89515) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -7.54300 LUMO: -0.02449 factor:1 | -1 (0.86377) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (1.02609) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.98244 LUMO: -0.95784 factor:1 | -1 (0.66709) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.96884 LUMO: -1.12383 factor:1 | -1 (0.88905) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.50420) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.29466) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.04533) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.39206) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.99333 LUMO: -1.33880 factor:1 | -1 (1.04660) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.63958 LUMO: -1.39322 factor:1 | -1 (0.81645) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.65411) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.01581) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-0.79016) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-0.69351) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.47661) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (0.24213) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.06553) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.19385) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.15837) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.14033) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.05597) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-0.35127) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-0.37448) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.15146) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.19494) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.10817) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (0.98606) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (1.13167) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -6.38379 LUMO: 0.58232 factor:1 | -1 (1.11376) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -7.42871 LUMO: 0.40273 factor:1 | -1 (1.37374) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -6.54978 LUMO: 0.26395 factor:1 | -1 (0.92908) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-0.78595) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.52610) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.84342) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-0.11480) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.15845) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.31391) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.95251 LUMO: -1.09118 factor:1 | -1 (0.12087) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.03148) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.01328) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (0.28482) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.52257 LUMO: -1.11022 factor:1 | -1 (0.16860) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.75114 LUMO: -1.09934 factor:1 | -1 (0.41963) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.02109) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (0.82423) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (0.62858) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (0.69354) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (0.72731) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (1.02127) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (0.88181) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.65871) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.42953) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (0.45832) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (0.73346) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -7.12938 LUMO: -0.23674 factor:1 | -1 (0.65628) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.14705 LUMO: -0.20409 factor:1 | -1 (0.98244) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.87855) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (1.00845) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (1.16865) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.87800) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -5.94025 LUMO: -0.17687 factor:1 | -1 (0.63952) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -5.62187 LUMO: 0.05714 factor:1 | -1 (0.58592) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -7.03414 LUMO: -1.04492 factor:1 | -1 (0.86037) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.75387 LUMO: -2.02181 factor:1 | -1 (0.64083) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.55250 LUMO: -0.75648 factor:1 | -1 (0.74325) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.54341) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (0.04316) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-0.12223) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.17037) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.10313) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.18926) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.13187) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.64382) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.89988) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (1.08073) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (1.25869) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (0.95966) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (0.82935) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (0.87169) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.56883 LUMO: -0.97689 factor:1 | -1 (0.91594) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.66679 LUMO: 0.56055 factor:1 | -1 (1.15597) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.75931 LUMO: 0.32926 factor:1 | -1 (0.95953) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.53617 LUMO: -1.06397 factor:1 | -1 (1.05610) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.78108 LUMO: 0.42722 factor:1 | -1 (1.36503) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -7.05319 LUMO: 0.61498 factor:1 | -1 (0.70992) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.78380 LUMO: 1.49391 factor:1 | -1 (1.04399) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.71408) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.87759) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (1.08358) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (1.38408) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.88840) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.70135) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (0.76132) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.95115) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.94859) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (1.30408) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (1.13265) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -7.00965 LUMO: -1.23268 factor:1 | -1 (1.10935) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (1.38130) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (0.84393) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (0.54537) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.94162 LUMO: -1.01771 factor:1 | -1 (0.77874) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -6.82189 LUMO: -0.92791 factor:1 | -1 (0.63296) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.92258 LUMO: -1.73881 factor:1 | -1 (0.54741) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.50896 LUMO: -1.60819 factor:1 | -1 (0.48504) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (0.77441) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (0.82168) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.57234) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.87338) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (0.62888) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (0.58428) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -7.52667 LUMO: -0.74287 factor:1 | -1 (0.79384) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (0.93044) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (0.84853) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (0.73109) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -6.97428 LUMO: -0.60681 factor:1 | -1 (0.68575) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.78380 LUMO: -0.88981 factor:1 | -1 (0.88638) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.85999 LUMO: 0.07891 factor:1 | -1 (1.07365) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (1.34941) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (0.82148) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.15657) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-0.18044) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.16496) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (0.25747) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (0.03195) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -5.98106 LUMO: -0.37824 factor:1 | -1 (0.12136) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -7.06408 LUMO: -1.12927 factor:1 | -1 (0.04991) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.70761 LUMO: -0.98505 factor:1 | -1 (0.61171) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -7.00965 LUMO: -0.42722 factor:1 | -1 (0.86178) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -5.96201 LUMO: -0.59049 factor:1 | -1 (0.82755) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.34570 LUMO: -1.68438 factor:1 | -1 (1.00772) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.97156 LUMO: -1.85854 factor:1 | -1 (1.05270) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -5.91848 LUMO: -2.51433 factor:1 | -1 (1.11251) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.39195 LUMO: -1.66262 factor:1 | -1 (1.27836) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (0.86257) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (0.88927) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (0.00623) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (0.15881) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-0.28096) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (0.37007) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (0.33059) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.23396) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (0.20615) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.07355) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.07984) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (0.17244) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (0.22849) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (0.45372) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.33734) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (0.28215) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.00988) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.21062) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.70761 LUMO: 0.28028 factor:1 | -1 (0.16202) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.08531) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.20742) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.58257) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-1.36370) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.37867) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.39639) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.22277) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-1.18459) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.80265) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.18391) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.98709) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-0.19875) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.78924 LUMO: -1.03675 factor:1 | -1 (0.23021) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-0.94709) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.05499) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.20637) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -7.20830 LUMO: 0.11429 factor:1 | -1 (0.16520) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.39846) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-0.11910) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-0.22177) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-0.26776) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.14207) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.58559) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.39320) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.43106) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.40208) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (0.97411) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (0.81354) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (0.96394) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.80285 LUMO: -0.60954 factor:1 | -1 (0.76842) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.10776) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-0.82456) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.75805) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.12245) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.60031) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.76203 LUMO: -2.13609 factor:1 | -1 (0.04482) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.15026) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.07208) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.04231) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.08607) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.66951 LUMO: -1.23812 factor:1 | -1 (0.27786) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.78380 LUMO: -1.27894 factor:1 | -1 (0.13946) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (0.17350) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -7.77974 LUMO: -0.26395 factor:1 | -1 (0.34735) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.04716) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.59876 LUMO: -0.91158 factor:1 | -1 (0.82812) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -4.67219 LUMO: -0.67756 factor:1 | -1 (0.76039) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.70489 LUMO: -0.65579 factor:1 | -1 (0.96309) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.62325 LUMO: -0.60409 factor:1 | -1 (0.75669) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.20147 LUMO: 0.15238 factor:1 | -1 (0.90802) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.43549 LUMO: -0.07075 factor:1 | -1 (0.76543) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -7.02054 LUMO: 0.13061 factor:1 | -1 (0.99126) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (0.78548) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.74842 LUMO: -0.99594 factor:1 | -1 (0.89191) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.35658 LUMO: 0.41633 factor:1 | -1 (0.94864) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.75049) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.51713 LUMO: -0.05987 factor:1 | -1 (0.92252) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.95052) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.90195) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.97945) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.84502) | 1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.90091) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (0.69803) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -7.36612 LUMO: -0.12245 factor:1 | -1 (0.80342) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (0.92445) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (1.23839) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.87087 LUMO: -0.08436 factor:1 | -1 (1.00508) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.81041) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.96339 LUMO: 0.65307 factor:1 | -1 (1.01724) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (0.80320) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.88747) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.97958) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (0.77607) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.91169 LUMO: 0.08163 factor:1 | -1 (0.70725) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (0.24702) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (0.16389) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.31255) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (0.21209) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (0.12637) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.00977) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.14969) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (0.24648) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-0.24455) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-1.17311) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.95428) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.20968) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-0.28817) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-0.80535) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-0.19663) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.99161) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.05118) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-0.02762) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.84080) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-0.24332) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-0.06621) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.02544) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-0.12732) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.19565) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.04678) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (0.24428) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.25391) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.83253) | 1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (0.81640) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (0.86040) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (1.23132) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (1.04786) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.96312) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (1.29692) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (1.09591) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.93909) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (1.03686) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-0.40959) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-0.14213) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-1.18146) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.09314) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.96486) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (0.01995) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (1.33575) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (1.12212) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (0.96677) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.62077) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.58899) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.98788 LUMO: -1.16737 factor:1 | -1 (0.20966) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.47816) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.95251 LUMO: 0.66396 factor:1 | -1 (0.33715) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.31105) | 1 | 1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.66769) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -7.04503 LUMO: -1.08301 factor:1 | -1 (0.11497) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.09377) | -1 | -1 |
| G: -6290.84798 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.01649) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-1.44868) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-1.94806) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-3.84078) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-3.28099) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-2.90754) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-1.86145) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-2.59999) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-2.68555) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-3.30850) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-2.61605) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-3.17190) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-3.20218) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.89394) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-3.28254) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-2.74827) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-2.79091) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-2.79820) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-2.85309) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-1.91862) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.90700) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.81712) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.92224) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-1.90730) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.66117) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-3.88423) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-3.08289) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-1.74705) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-3.15998) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-3.21916) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-2.58111) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-2.74576) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-2.69515) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-1.74066) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.77405) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.87263) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-2.06594) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-2.07514) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-2.01566) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-2.17511) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-1.98170) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-2.58688) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-2.72073) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-2.49869) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.87073) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.84956) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-2.02107) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-1.89867) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.95601) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-1.88991) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-2.59708) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-2.80626) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-2.74677) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.97021) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-2.45735) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-2.58290) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-2.54467) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-2.61746) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-2.38467) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-2.39770) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-2.67379) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-3.90004) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-3.13306) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-2.91592) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-3.27149) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.90224) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-3.41751) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-2.87175) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.96412) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.81007) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.58963) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-1.73579) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.88621) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-2.46279) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-2.51754) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-2.69085) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.85390) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-2.60505) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.55298) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-1.54234) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-3.75914) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-2.85616) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.51472) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-3.12705) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-3.23957) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-2.46451) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-2.48342) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.86393) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-2.96797) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-2.87064) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-3.40893) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-2.09081) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-2.61540) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.44418) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.20815) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-2.15879) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-2.12820) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-2.32157) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-2.17223) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.99544) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-2.04442) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-2.74566) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-2.69951) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-2.56247) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-2.85224) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-2.69423) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-2.73360) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-1.83794) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-2.66495) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-2.81175) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-2.65893) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-2.62326) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-2.89053) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-2.77668) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-2.88849) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-2.70193) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-2.81749) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-2.61950) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-2.54723) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-1.92779) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-2.64057) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-2.56832) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-2.58884) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-2.68299) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-2.79850) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-2.91116) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-2.07645) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-2.52024) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-2.18657) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-2.47371) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-2.22529) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-2.59180) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-2.66840) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-2.66195) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-2.63967) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-2.24254) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-2.20722) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-2.46560) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-2.34655) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-2.30578) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.93266) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-2.12744) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-2.11383) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-2.05517) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-1.68365) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-2.19275) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-1.82060) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-2.55847) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-3.09451) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-3.05600) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-3.62295) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-3.45489) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-3.13538) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-2.74190) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-3.05864) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-3.01069) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-3.26300) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-3.59691) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-3.59620) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-3.75384) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-3.11440) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-3.80636) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-3.65675) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-2.85385) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-3.08738) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-3.77041) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-3.64075) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-3.30866) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-3.04577) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-2.75638) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-1.61494) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-1.47948) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-2.64293) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-2.69224) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-2.88552) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-2.57901) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-1.99800) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-1.85628) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-1.77630) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-1.95253) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-1.94877) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-1.65271) | 1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-3.24624) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-3.68818) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-1.75470) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-3.08958) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-2.43262) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-2.75442) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-3.32512) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-2.97513) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-2.71665) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-2.63137) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-2.78160) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-2.41191) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-2.75777) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-3.05489) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-2.62827) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-1.47693) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-1.66351) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-1.19638) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-1.76575) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-2.53153) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-3.14044) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-2.68155) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-2.38804) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-3.06797) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-2.99608) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-3.15543) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-2.79374) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-2.62723) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-2.56973) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-2.91654) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-2.62486) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-2.98185) | 1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-3.02914) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-3.17464) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-2.86046) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.71162) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.63165) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-1.81130) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.51984) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.79922) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-2.60122) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-3.17214) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-2.54571) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-3.40053) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-2.74568) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-3.08536) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-2.52930) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-2.38560) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-2.61817) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-2.67406) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-2.40160) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-2.30698) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-2.09528) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-2.25019) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.54953) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-1.73372) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.88183) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-2.04480) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.91968) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.53467) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.61336) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.94765) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.58797) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-1.82667) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-1.49309) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-1.97808) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-1.66340) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-1.83214) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.82880) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.50171) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.40087) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-1.58898) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-1.62634) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-1.72945) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-1.63962) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-1.45061) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-1.94635) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-1.86716) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.99998) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-1.86678) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-1.61263) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-1.72322) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-1.76316) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.39820) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.46444) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.62547) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-1.66515) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-1.76085) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-1.74324) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-1.87778) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-1.62275) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-1.66038) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-2.30113) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-2.40649) | 1 | 1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-2.49996) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-2.54894) | -1 | -1 |
| G: -6288.43487 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-2.18731) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-2.19435) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-2.55931) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-2.35787) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-2.90365) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-3.00076) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-3.77544) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-3.75463) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-3.03665) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-3.60499) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-3.47149) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-2.80329) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-3.28988) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-2.65809) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-2.66522) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-2.56217) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-2.91121) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-2.59801) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.81383) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-1.81794) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.50278) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-1.91253) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-1.69943) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.48993) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.74474) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-1.59173) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-3.06991) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-3.60494) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-2.73771) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-3.72012) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-3.42817) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.46912) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.68596) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-1.47252) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-3.07910) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-2.30910) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-2.48396) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-3.25688) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-2.38951) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-3.00120) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-2.16635) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-2.66163) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-2.71412) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-2.48598) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-2.53899) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-2.63251) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.47180) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-2.49058) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-2.29278) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-2.90068) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-2.67164) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-2.87518) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-3.44668) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-2.62941) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-3.22360) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-2.48445) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-2.64579) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-2.49898) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-2.33939) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.65013) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-1.48672) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.48552) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.61562) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.65932) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-1.37170) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.38321) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-1.62351) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-1.43899) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-1.21395) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-1.55946) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-1.44917) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-2.89401) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-3.74034) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-2.67504) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.37521) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.52765) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-1.50234) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-3.10879) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-2.42742) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-2.95970) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.34951) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-2.50802) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-3.22928) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-2.59556) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-3.38550) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-2.43700) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.86322) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.72754) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.91497) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-1.73105) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.56691) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.90169) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-2.17931) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-2.12967) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-2.00885) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.63513) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-2.16611) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.90297) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-2.04624) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.95000) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-2.05441) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-2.07163) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-1.89179) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.73288) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.90047) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-1.88344) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.57086) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.91489) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-1.94831) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-2.57273) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-2.61262) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-2.81439) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-2.79472) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-2.72370) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-2.66119) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-2.00006) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-2.13109) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.99114) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-2.24431) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-2.52309) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-2.44424) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-2.50652) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-2.56767) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-2.45422) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-2.18801) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-2.69474) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-2.62922) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-2.48435) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-2.28987) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-2.30532) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-2.53553) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-2.56750) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-2.30622) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-2.14167) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-2.49313) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-2.55085) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.82986) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.76749) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.59285) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.41401) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.33986) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.97239) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-1.65794) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-1.81631) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.89949) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.70692) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.54332) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.79051) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.69116) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-1.82292) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.61851) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.47361) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.75767) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-2.44356) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-2.47994) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-2.40492) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-2.05198) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-2.47270) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-2.27476) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.95000) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.72302) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-1.80235) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.45314) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-1.87484) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-1.54738) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-1.39562) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-1.67100) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.64496) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-1.83002) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.94578) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-2.03190) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.78471) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-1.74615) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-1.62191) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.74101) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-1.75492) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.49660) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-1.81451) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-1.46781) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-1.57078) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-1.38569) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.20394) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.70621) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.37450) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-1.96518) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-1.85723) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-2.34919) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-2.37966) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-2.24083) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-2.56056) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-1.60983) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-1.46109) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.17137) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.27273) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-0.96845) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.61011) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-1.37491) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-2.05114) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-1.92466) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-1.83176) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-2.02292) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.74264) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.84376) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-2.59833) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-2.71668) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-2.75676) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-2.50535) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-2.55444) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.93345) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-1.99979) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.83307) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-1.72147) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.62784) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.55148) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.58939) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.31537) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.68251) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-2.55343) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-2.74895) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-2.28867) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-2.71804) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-2.56299) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-2.00518) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-1.74569) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-1.88189) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.57255) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-1.37782) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.59769) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-1.80482) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-1.95568) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-1.64735) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.75875) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.82205) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-1.39548) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-1.39834) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-1.12987) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-1.53872) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-1.75045) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-1.74289) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-2.72394) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-2.78743) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-2.54173) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-2.57675) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-2.40742) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-2.44045) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-2.39501) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-2.58084) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-2.48228) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-2.21691) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-2.55809) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-2.45673) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-2.47828) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-2.30802) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-2.52299) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-2.55915) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-2.71409) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-2.54878) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-2.36867) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-2.30034) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-2.59237) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-2.60214) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-2.63768) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-2.43164) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-2.60154) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-2.22929) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-2.19158) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-2.52013) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-2.37177) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-1.65279) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.76547) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.79350) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.90776) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-1.52890) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-1.58610) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-1.63649) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-1.82509) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-1.71892) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.68866) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-1.53777) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-2.65273) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-2.66870) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-2.41504) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-2.74468) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-2.50802) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-2.35661) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-2.17326) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-2.57986) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-2.37017) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-2.54299) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-2.49809) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-2.30494) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-2.20709) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-2.59444) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-2.45117) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-2.14986) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-2.10543) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-1.99274) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.66419) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-2.39490) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-2.25963) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-2.05582) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-2.43991) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-2.26260) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-2.40097) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-2.61763) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-2.17022) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-2.10652) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-2.19076) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-2.55629) | -1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-2.35558) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-2.42734) | 1 | -1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-2.33904) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-2.56299) | 1 | 1 |
| G: -6288.43487 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-2.06001) | 1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.93304) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-2.03432) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-1.66942) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-2.31572) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-2.11215) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-2.10777) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-2.02619) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.83963) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-2.31125) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-3.00501) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-3.78211) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-2.65926) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-2.80103) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-3.00607) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-2.59656) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-3.09587) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-3.60366) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-3.32137) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-3.77958) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-2.62116) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-2.43760) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-2.25509) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-3.72097) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-2.93905) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-3.86657) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-2.56217) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-3.33201) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-3.08716) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-2.87309) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-1.72566) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.59459) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-3.13930) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-2.59752) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-2.98977) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-2.54163) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-2.48554) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-2.59542) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-2.51733) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.65872) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-2.44448) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-2.31202) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-2.38094) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-2.09054) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-2.83311) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-3.02392) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-2.82623) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-3.05285) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-3.63283) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-2.85918) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-3.32964) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-3.41647) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-2.69643) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-3.26156) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-2.54312) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-2.61752) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-2.82095) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-2.66506) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-2.43656) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-2.45207) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-1.80398) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-1.58324) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-1.50152) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-1.76131) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-1.71151) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-1.31333) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-1.58822) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.51796) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.54933) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-1.38702) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-1.74602) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-1.52406) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-2.91731) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-3.70777) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-3.45843) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-2.80517) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.36650) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.59666) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-3.06721) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-2.39730) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-3.20327) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-3.10662) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-2.88971) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-2.17098) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-2.47863) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-2.60696) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-2.57148) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-2.55343) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-2.46908) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-2.76438) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-2.78759) | 1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-2.56456) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-2.60805) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-2.30494) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.42705) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-1.28144) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.29934) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-1.03937) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-1.48403) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-3.19905) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-2.93921) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-3.25652) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-2.52791) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-2.25465) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-2.09920) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-2.29223) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-2.44459) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-2.42638) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-2.12828) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-2.24450) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.99348) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-2.43419) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-1.58887) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.78452) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.71957) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-1.68580) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.39184) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.53129) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.75440) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.98357) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.95478) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.67965) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.75682) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.43067) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.53456) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.40465) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.24446) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.53510) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.77358) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.82719) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.55274) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.77228) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.66985) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.86969) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-2.36995) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-2.53534) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-2.24274) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-2.30997) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-2.22385) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-2.28124) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.76928) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.51323) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-1.33238) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-1.15442) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-1.45344) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-1.58376) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-1.54142) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-1.49717) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-1.25714) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.45358) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.35700) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.04807) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.70319) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.36911) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.69902) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.53551) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-1.32952) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.02903) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.52471) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.71176) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.65179) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.46196) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.46452) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.10903) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.28046) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.30375) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.03180) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.56917) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.86774) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-1.63437) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-1.78014) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-1.86569) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-1.92806) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-1.63870) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-1.59143) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.84077) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-1.53973) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-1.78422) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-1.82882) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-1.61927) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-1.48267) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.56457) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.68202) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.72735) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.52672) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.33945) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.06369) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.59162) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-2.56968) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-2.59354) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-2.57806) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-2.15563) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-2.38116) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-2.29174) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-2.36320) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-1.80139) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.55132) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-1.58555) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-1.40539) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.36041) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.30060) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.13474) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.55053) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-1.52384) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-2.40687) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-2.25430) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-2.69406) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-2.04303) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-2.08251) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-2.17914) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-2.20695) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-2.33955) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-2.33327) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-2.24067) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-2.18461) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.95938) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-2.07577) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-2.13095) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-2.42298) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-2.20249) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-2.25109) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-2.49841) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-3.62053) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-2.99567) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-3.77680) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-2.79178) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-2.80949) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-3.63588) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-3.59770) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-3.21576) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-3.59702) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-3.40020) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-2.61186) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-2.18290) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-3.36020) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-2.46810) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-2.61948) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-2.24791) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-2.81156) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-2.53221) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-2.63488) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-2.68087) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-2.55518) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-2.99869) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-2.80631) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-2.84416) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-2.81518) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.43899) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.59957) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-1.44917) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.64468) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-2.52086) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-3.23767) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-3.17116) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-2.53556) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-3.01342) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-2.36829) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-2.56337) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-2.48519) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-2.45542) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-2.49918) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.13525) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-2.27365) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.23961) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-2.06575) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-2.46026) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.58498) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.65271) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.45001) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-1.65641) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.50509) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.64768) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.42185) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-1.62762) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.52120) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-1.46446) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.66262) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.49059) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.46258) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.51116) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.43366) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.56808) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.51219) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.71508) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.60969) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.48865) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.17472) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.40803) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.60270) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.39586) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.60991) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.52563) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.43352) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.63704) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-1.70585) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-2.16608) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-2.24921) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-2.10056) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-2.20102) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-2.28674) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-2.42287) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-2.56280) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-2.16662) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-2.65765) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-3.58622) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-3.36738) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-3.62279) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-2.70127) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-3.21845) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-2.60974) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-3.40472) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-3.46428) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-2.44073) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-3.25391) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-2.65643) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-2.47931) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-2.38766) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-2.54043) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-2.60876) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-2.45988) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-2.16883) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-2.66702) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-1.58057) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-1.59671) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-1.55271) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-1.18179) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-1.36525) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-1.44999) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.11618) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.31719) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.47401) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.37624) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-2.82269) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-2.55523) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-3.59457) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-3.50624) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-3.37797) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-2.39316) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-1.07735) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-1.29099) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-1.44634) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-3.03388) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-3.00210) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-2.20344) | 1 | 1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-2.89126) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-2.07596) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-2.10205) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-3.08079) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-2.29814) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-2.31934) | -1 | -1 |
| G: -6288.43487 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-2.42960) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.17570) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.67509) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-2.56780) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-2.00801) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-1.63456) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.58847) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-1.32702) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-1.41257) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-2.03552) | 1 | 1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-1.34307) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-1.89892) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-1.92921) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.62096) | 1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-2.00956) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-1.47529) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-1.51793) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-1.52523) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-1.58011) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.64564) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.63403) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.54415) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.64926) | 1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.63432) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.38820) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-2.61126) | -1 | -1 |
| G: -6289.70785 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.80991) | 1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.47408) | 1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-1.88700) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.94619) | 1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.30813) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-1.47279) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-1.42218) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.46768) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.50107) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.59966) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.79297) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.80216) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.74268) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.90214) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.70872) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.31390) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.44775) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-1.22571) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.59775) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.57658) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.74810) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.62570) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.68303) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.61694) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-1.32411) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-1.53328) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-1.47380) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.69724) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.18438) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.30993) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.27170) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.34449) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.11169) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-1.12473) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.40081) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-2.62707) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-1.86009) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.64294) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.99851) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.62926) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-2.14453) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-1.59878) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.69114) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.53710) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-0.31666) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-0.46281) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.61324) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.18982) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.24457) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-1.41788) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.58093) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.33208) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.28001) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-0.26937) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-2.48617) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.58319) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-0.24175) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.85407) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.96659) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-1.19153) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-1.21044) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.59095) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-1.69500) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-1.59766) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-2.13596) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.81784) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-1.34242) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.17121) | 1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-0.93517) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.88581) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.85523) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.04859) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-0.89925) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.72246) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.77144) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-1.47268) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.42653) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-1.28949) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.57927) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-1.42125) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.46063) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.56496) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-1.39197) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.53878) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.38596) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.35028) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.61755) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-1.50370) | 1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.61551) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.42895) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-1.54452) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.34653) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-1.27425) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.65481) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.36759) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-1.29534) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-1.31586) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.41001) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.52552) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.63818) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.24726) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-0.91360) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.20073) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.95232) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-1.31883) | -1 | -1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.39543) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.38898) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-1.36669) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.96957) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.93425) | 1 | 1 |
| G: -6289.70785 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.19262) | -1 | -1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-1.07357) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.03281) | -1 | -1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.65969) | -1 | -1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.85446) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.84086) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.78219) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.41067) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.91977) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.54763) | -1 | -1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-1.28549) | 1 | 1 |
| G: -6289.70785 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-1.82153) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.78303) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.34998) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-2.18192) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.86240) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.46893) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.78567) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.73772) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.99002) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-2.32393) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-2.32323) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-2.48086) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.84142) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-2.53338) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-2.38377) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.58087) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.81440) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-2.49743) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-2.36777) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-2.03568) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.77279) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.48340) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.34197) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.20651) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.36996) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.41926) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.61255) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.30604) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.72502) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.58330) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.50333) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.67955) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.67579) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.37973) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.97326) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-2.41520) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.48172) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.81660) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.15964) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.48144) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.05215) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.70215) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.44367) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.35839) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.50863) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.13893) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.48479) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.78191) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.35529) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.20395) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.39054) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.18653 LUMO: 0.59321 factor:1 | -1 (0.07660) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.49277) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.25855) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.86746) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.40857) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.11507) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.79500) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.72311) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.88246) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.52076) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.35426) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.29676) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.64357) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.35189) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.70888) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.75617) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.90167) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.58749) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.43865) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.35867) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.53832) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.24686) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.52624) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.32824) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.89916) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.27273) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-2.12755) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.47271) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.81239) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.25632) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.11262) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.34519) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.40109) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.12862) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.03401) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.82230) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.97722) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.27655) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.46074) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.60885) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.77182) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.64671) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.26169) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.34039) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.67468) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.31500) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.55370) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.22011) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.70510) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.39043) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.55917) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.55582) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.22874) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.12789) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.31601) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.35337) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.45647) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.36665) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.17764) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.67337) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.59419) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.72701) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.59381) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.33965) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.45024) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.49019) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.12523) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.19146) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.35250) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.39217) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.48787) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.47027) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.60480) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.34978) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.38741) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.02816) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.13352) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.22699) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.27597) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.91433) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.92138) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.28634) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.08489) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.63067) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.72779) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-2.50247) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.48165) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.76368) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-2.33202) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-2.19852) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.53031) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-2.01691) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.38511) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.39224) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.28919) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.63823) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.32503) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.54085) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.54496) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.22980) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.63955) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.42646) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.21696) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.47176) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.31875) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.79693) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-2.33196) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.46473) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.44715) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.15520) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.19614) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.41299) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.19954) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.80613) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.03613) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.21099) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.98390) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.11654) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.72822) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.89338) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.38865) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.44114) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.21300) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.26601) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.35954) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.19882) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.21760) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.01980) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.62770) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.39867) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.60221) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.17370) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.35643) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.95062) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.21148) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.37281) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.22601) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.06641) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.37715) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.21375) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.21255) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.34265) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.38635) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.09872) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.11023) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.35054) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.16602) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -7.52395 LUMO: 0.26395 factor:1 | -1 (0.05902) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.28648) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.17619) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.62104) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-2.46737) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.40207) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.10223) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.25467) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.22936) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.83582) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.15444) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.68672) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.07654) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.23504) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.95631) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.32258) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-2.11253) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.16402) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.59024) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.45457) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.64200) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.45808) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.29394) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.62872) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.90633) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.85670) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.73588) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.36216) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.89313) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.63000) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.77327) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.67702) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.78143) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.79865) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.61881) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.45990) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.62749) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.61046) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.29788) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.64192) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.67533) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.29975) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.33964) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.54142) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.52174) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.45072) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.38822) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.72709) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.85811) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.71816) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.97134) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.25012) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.17126) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.23355) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.29469) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.18125) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.91504) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.42177) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.35624) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.21137) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.01689) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.03235) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.26255) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.29453) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.03324) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.86870) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.22016) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.27787) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.55688) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.49451) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.31987) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.14104) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.06689) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.69941) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.38496) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.54333) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.62651) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.43394) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.27035) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.51753) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.41818) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.54994) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.34553) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.20063) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.48469) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.17058) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.20696) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.13194) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.77901) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.19972) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.00179) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.67702) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.45005) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.52937) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.18017) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.60186) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.27440) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.12264) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.39802) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.37198) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.55704) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.67280) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.75893) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.51174) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.47318) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.34893) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.46804) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.48194) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.22362) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.54153) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.19483) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.29780) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.11271) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.06904) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.43323) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.10153) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.69220) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.58426) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.07621) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.10669) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.96785) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.28759) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.33685) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.18811) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (0.10161) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.00024) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (0.30452) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.66287) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.10193) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.77816) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.65169) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.55879) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.74995) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.46967) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.57079) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-1.32536) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.44370) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-1.48378) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.23238) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.28147) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-0.66047) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.72682) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.56009) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.44850) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.35486) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-0.27851) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.31641) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.04240) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.40953) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-1.28046) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-1.47597) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-1.01569) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-1.44506) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-1.29001) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.73220) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.47272) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.60891) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.29957) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.10485) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-0.32471) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.53185) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.68271) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.37437) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.48578) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.54907) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-0.12251) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-0.12536) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.14310) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.26575) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.47748) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.46991) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.45097) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-1.51445) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-1.26876) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-1.30378) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-1.13444) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-1.16748) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-1.12203) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-1.30786) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-1.20930) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.94394) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-1.28511) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-1.18375) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-1.20530) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-1.03504) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-1.25001) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-1.28617) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-1.44112) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-1.27581) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-1.09569) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-1.02737) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-1.31940) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-1.32917) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.36471) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.15866) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-1.32857) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-0.95632) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.91860) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-1.24715) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.09880) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-0.37982) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.49250) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-0.52053) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-0.63479) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.25592) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-0.31312) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.36352) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.55212) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.44594) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.41568) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.26479) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-1.37975) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-1.39573) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.14206) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.47170) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-1.23504) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-1.08364) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.90029) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-1.30688) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.09719) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-1.27001) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-1.22511) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.03196) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.93411) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-1.32147) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-1.17820) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.87689) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.83245) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.71977) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.39122) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-1.12193) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.98666) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.78284) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.16693) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.98962) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-1.12799) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-1.34465) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.89724) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.83354) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.91779) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-1.28332) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-1.08260) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-1.15436) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-1.06606) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-1.29001) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.78703) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.66007) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.76135) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.39644) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.04274) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.83917) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-0.83479) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.75321) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.56665) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-1.03828) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-1.73203) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-2.50913) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-1.38628) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-1.52806) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-1.73309) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-1.32359) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-1.82289) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-2.33068) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-2.04839) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-2.50660) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.34819) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.16462) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.98211) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-2.44799) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.66607) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-2.59360) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-1.28919) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-2.05903) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-1.81418) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-1.60011) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.45269) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-0.32161) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-1.86632) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.32454) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.71679) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.26865) | 1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.21257) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-1.32245) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-1.24435) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-1.38574) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-1.17150) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-1.03904) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.10797) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.81757) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-1.56014) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-1.75094) | -1 | -1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-1.55325) | 1 | 1 |
| G: -6289.70785 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.77987) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.35985) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.58621) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-2.05666) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.14350) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.42345) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.98858) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.27015) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.34454) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.54797) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.39208) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.16359) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.17910) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.53100) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.31026) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.22855) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.48834) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.43854) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.04035) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.31524) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.24498) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.27636) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.11404) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.47304) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.25108) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.64433) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-2.43479) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-2.18546) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.53219) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.09353) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.32368) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.79424) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.12432) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.93029) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.83364) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.61674) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.89800) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.20565) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.33398) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.29850) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.28046) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.19610) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.49140) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.51461) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.29159) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.33507) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.03196) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.15407) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.00846) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.02637) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.82734 LUMO: -0.60137 factor:1 | -1 (0.23361) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.21105) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.92608) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.66623) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.98355) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.25493) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.98168) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.82622) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.01926) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.17161) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.15341) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.85531) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.97153) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.72050) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.16122) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.31590) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.51155) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.44659) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.41282) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.11886) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.25832) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.48142) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.71060) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.68181) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.40667) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.48385) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.15769) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.26158) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.13168) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.71305 LUMO: -0.49525 factor:1 | -1 (0.02852) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.26213) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.50061) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.55421) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.27976) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.49930) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.39688) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.59672) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.09697) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.26236) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.96976) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.03700) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.95087) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.00826) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.49631) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.24025) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.05940) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.52529 LUMO: 1.70071 factor:1 | -1 (0.11856) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.18047) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.31078) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.26844) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.22419) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.01584) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.18060) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.08403) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.22490) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.43021) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.09614) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.42605) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.26254) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.05655) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.56883 LUMO: 1.81228 factor:1 | -1 (0.24395) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.25173) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.43878) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.37881) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.18898) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.19154) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (0.16395) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.00748) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.03078) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.24117) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.29620) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.59476) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.36139) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.50717) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.59272) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.65509) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.36572) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.31845) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.56779) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.26675) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.51125) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.55585) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.34629) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.20969) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.29160) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.40904) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.45438) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.25375) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.06648) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.20928) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.31865) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.29670) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.32057) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.30509) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.88266) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.10818) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.01877) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.09022) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.52842) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.27835) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.31258) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.13241) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.08743) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.02762) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.13823) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.27756) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.25086) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.13390) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.98132) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.42109) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.77006) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.80954) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.90617) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.93398) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.06658) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.06029) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.96769) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.91164) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.68641) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.80279) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.85798) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.15001) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.92951) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.97811) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.22544) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.34755) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.72270) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.50383) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.51880) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.53652) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-2.36290) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-2.32472) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.94278) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-2.32404) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-2.12722) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.33888) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.90992) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-2.08722) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.19512) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.34650) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.97493) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.53859) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.25923) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.36190) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.40789) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.28220) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.72572) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.53333) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.57119) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.54221) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.16602) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.32659) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.17619) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.37171) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.24789) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.96469) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.89818) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.26258) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.74044) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.09531) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.29039) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.21221) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.18244) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.22620) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.86227) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.00067) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.96663) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.79278) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.18729) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.31201) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.37973) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.17704) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.38344) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.23211) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.37470) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.14887) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.35465) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.24822) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.19149) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.38964) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.21761) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.18961) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.23818) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.16068) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.29511) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.23922) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.44210) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.33671) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.21568) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (0.09826) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.13505) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.32972) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.12289) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.33693) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.25266) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.16055) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.36406) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.43288) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.89310) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.97624) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.82758) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.92804) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.01376) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.14990) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.28982) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.89365) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.38468) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-2.31324) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-2.09441) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-2.34981) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.42830) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.94548) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.33676) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-2.13174) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-2.19131) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.16775) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.98093) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.38345) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.20634) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.11469) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.26745) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-1.33578) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.18691) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.89585) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-1.39404) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.30760) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.32373) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.27973) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.09673 LUMO: 2.35106 factor:1 | -1 (0.09119) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.09227) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.17701) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.15679) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.04422) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.20104) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.10327) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.54972) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.28225) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-2.32159) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-2.23327) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-2.10499) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.12018) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.87632 LUMO: 1.92657 factor:1 | -1 (0.19562) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.01801) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.17336) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.76090) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.72912) | 1 | 1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.93047) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.61829) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.80298) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.82908) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.80782) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.02516) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.04636) | -1 | -1 |
| G: -6289.70785 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.15662) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.75495) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.25434) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-3.14705) | 1 | 1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-2.58726) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-2.21381) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.16772) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.90627) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.99182) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-2.61477) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.92232) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-2.47817) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.50845) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.20021) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-2.58881) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-2.05454) | 1 | 1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-2.09718) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-2.10447) | 1 | 1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-2.15936) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.22489) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.21327) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.12339) | 1 | 1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.22851) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.21357) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.96745) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-3.19051) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-2.38916) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.05333) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-2.46625) | -1 | -1 |
| G: -6289.12860 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-2.52543) | -1 | -1 |